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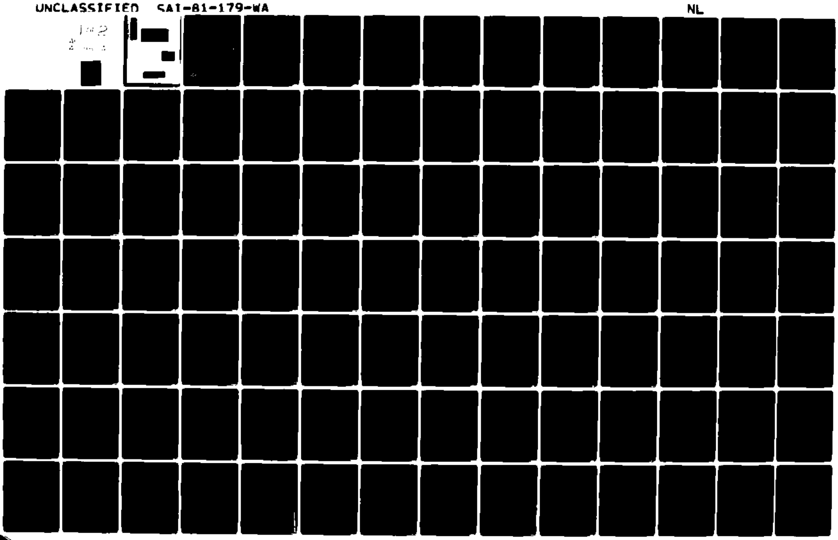

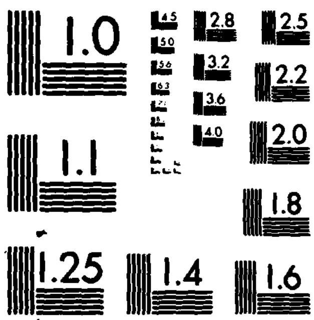

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REQUIREMENTS FOR AN HISTORICAL
STRATIFICATION FILE USING STD AND CTD DATA

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REQUIREMENTS FOR AN HISTORICAL STRATIFICATION FILE USING STD AND CTD DATA

SAI-81-179-WA

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Prepared for:

E. M. Stanley
NORDA Code 500
NSTL Station, MS 39529

Prepared by:

E. J. Molinelli
A. D. Kirwan

101

SCIENCE APPLICATIONS, INC.

1710 Goodridge Drive
McLean, Virginia 22102
703) 821-4300

408404

TABLE OF CONTENTS

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LIST OF TABLES

LIST OF FIGURES

Section 1
INTRODUCTION

The National Oceanographic Data Center (NODC) has an obligation to archive stratification data. This task involves coping with modern electronic STD and CTD measurements. The details of performing the modern measurements are examined, and the means by which NODC may cope with them are described, in this report. This report constitutes a preliminary step in defining a new system to automatically accept, store and disseminate STD/CTD data.

1.1 STRATIFICATION

Stratification is an important tool in the study of the oceans. In its narrowest sense, stratification is the vertical distribution of temperature, salinity and the resultant density. The vertical coordinate may be depth or pressure (the two parameters are related by the hydrostatic equation) but pressure is required for the calculation of _in situ_ density and other dynamic parameters. Temperature, salinity, density and pressure are of primary use. They indicate the location of water masses, which are unique combinations of temperature and salinity, that can be traced thousands of kilometers in some cases. The horizontal distribution of density stratification represents information about the distribution of gravitational forces that effect the vertical shear of horizontal velocities. Internal waves, which store vast amounts of kinetic energy in the ocean, have properties which depend upon the density stratification. For all these purposes a knowledge of stratification is required.

In a broader sense, stratification may refer to the vertical distribution of any parameter. The applications of such data are as varied as the number of parameters. For this report the term stratification will be used in its narrow sense with only occasional reference to some of the other, less frequently measured, parameters (such as dissolved oxygen, nutrients, sound velocity and horizontal velocity) whose vertical distributions are also of interest in present oceanographic research.

1.2 MEASUREMENTS

The technique for measuring the ocean stratification has undergone a radical change in the past two decades. Formerly, samples of salinity, temperature and pressure could be obtained only at a few, discreet locations in the vertical. These "classical" measurements involve instruments arranged on a cable. Temperature is determined by reversing thermometers. Salinity is determined from a titration for chloride on a water sample trapped in a water bottle (e.g., a Nansen bottle). Pressure is determined from a second reversing thermometer not "protected" from pressure effects. The entire process of deploying and reading the instruments and recording the data is time consuming and tedious. It has to be repeated for every station and for deep basins several times per station. (Throughout this report a station is taken to mean data representative of a single geographic position for a single point in time. It is understood that there is some breadth to both the space and time coordinates).

The past two decades have seen the development of electronic devices that can measure and record temperature, salinity and pressure continuously. Temperature measurements are based on platinum thermometers. Pressure is determined from strain gage transducers. Salinity is based on measurements of ocean water conductivity. The sensors are combined in a watertight unit that is lowered through the water and which transmits data to the ocean platform through a conducting cable. The various devices are called STDs, CSTDs and CTDs. With these instruments a station, which can now include thousands of observations, can be accumulated automatically and more rapidly than with the classical instruments. The popularity of these instruments is not surprising.

1.3 THE NATIONAL OCEANOGRAPHIC DATA CENTER

The National Oceanographic Data Center (NODC) is an element of the Environmental Data and Information Service (EDIS) of the National Oceanic and Atmospheric Administration (NOAA) of the United States Department of Commerce. According to its mission statement, NODC is "concerned with the development of a national marine data base, including acquisition, processing, storage, and retrieval of marine data and information generated by domestic and foreign activities..." (NOAA, 1978). As one facet of meeting the stated obligation, NODC has generated and continues to maintain a file of classically measured stratification data called the Serial Depth Data file. Data documentation, quality control and data management requirements for modern STD/CTD data are all sufficiently different, however, that the Serial Depth Data file can not be expanded to include them. To fulfill its mission NODC must develop a new system.

1.4 OUTLINE OF REPORT

The data documentation requirements for the new system are derived in this report based upon an examination of methods of data collection and methods of data processing. Although the observations from all STDs and CTDs provide relatively continuous density stratification information from electronic measurements transmitted to an ocean platform via cable, they have little else in common. They differ in actual vertical sampling interval, measurement accuracy, measurement noise, sampling procedure, digitization, salinity determination, inclusion of additional parameters, and instrument characteristics including type of conductivity cell and use of additional temperature sensors. These items will be defined and discussed in the following sections. Data quality depends upon the items summarized above, so that proper data documentation must accommodate all of them. Proper data documentation then allows a single data management system to handle STD/CTD data which is quite diverse in quality.

The quality control and data management requirements for the new system are derived from an examination of the uses to which disseminated data might be put and the techniques available for data quality control.

One section is devoted to each of the four subjects influencing the requirements for the new system: measurement techniques; processing techniques; the secondary user; and testing data. Throughout each section reference is made to the STD/CTD stratification archive NODC must create whenever points are presented that bear upon it. These points are pulled together as recommendations in the final section of this report.

Section 2
SUMMARY OF MEASUREMENT TECHNIQUES

This section describes ways in which STDs and CTDs have been used. It is essentially a historical treatment. In general, it is not an attempt to instruct the reader to follow a particular set of procedures.

2.1 INSTRUMENTS

According to the Ocean Science Committee's ad hoc Panel (1973), the majority of instruments in use in 1973 were made up of three models of STDs manufactured by Plessey Environmental Systems (now Grundy Environmental Systems, Inc.), the 9006, 9040 and 9060. Together they amounted to nearly 80% of the instruments in use among respondents to that survey. The remaining instruments were distributed among 15 other models, two by Plessey and 13 by other manufacturers. Ten of these models were uniquely represented in the survey. Since that time, the Neil Brown CTD, originally one of those singly-used instruments, has blossomed in popularity and is now one of the most widely used instruments. Moreover, Grundy presently has a new model, the 9051. Rather than deal explicitly with every instrument ever used, the characteristics of the 9006, 9040 and 9051 STDs, and the Neil Brown CTD are taken to be typical. The variability existing among these devices is taken to be typical of the variability in the data available to NODC.

Throughout this report the terms accuracy, resolution, precision, noise and repeatability are used to

assess data quality. If the same signal were measured repeatedly by an instrument or technique the measured values in general are distributed about a mean value with a variance s^2. The value of s is then a measure of the repeatability of that instrument or technique. In this report the term repeatability is used interchangeably with the terms noise level and precision. The difference between the distribution's mean value and the value of the signal according to some fixed standard is then the accuracy of the measurement. A separate property from either the accuracy or precision of an instrument or technique is its resolution. Measurements in general cannot be assigned values continuously in any range, but instead take on more or less closely spaced, but discreet values. The separation of possible values for the measurement is the resolution of the instrument or technique.

The manufacturer's specifications on sensor response times and data accuracy and precision for the devices are given in Table 2.1. Both accuracy and precision improve down the table.

Differences in these four instruments besides accuracy, precision and time response have some influence on the data. The salinity sensor of the STD is actually a conductivity sensor with electronic networks that suppress transients and attempt to compensate for the effects of temperature and pressure on the conductivity measurement. The temperatures used for this correction enter the network at three different points and come from three different sensors none of which has its measurements recorded. The original conductivity measurement is lost in the process. The 9051 now reports conductivity separately as do the

TABLE 2.1 MANUFACTURERS SPECIFICATIONS OF UNDERWATER UNIT

INSTRUMENT	PARAMETER	TIME CONSTANT (sec)	RANGE	ACCURACY	PRECISION*
PLESSEY 9006 (STD)	temperature	.35	-2 to 35°C	.02°C	not given
	pressure	not given	0 to 1500, 0 to 3000, 0 to 6000 dbar	.25% of full scale	not given
	salinity	.35	33 to 41°/oo	.03°/oo	.02°/oo
	sound velocity (optional)	not given	1400 to 1600 m sec^{-1}	.15 m sec^{-1}	not given
PLESSEY 9040 (STD)	temperature	.35	-2 to 35°C	.02°C	.004°C
	pressure	.02	0 to 1500, 0 to 3000, 0 to 6000 dbar	.25% of full scale	.02% of full scale
	salinity	.35	30 to 40°/oo	.02°/oo	.003°/oo
	sound velocity (optional)	.00007	1400 to 1600 m sec^{-1}	.15 m sec^{-1}	.07 m sec^{-1}
GRUNDY 9051 (CSTD)	temperature	.35 .05 (optional)	-2 to 35°C	.02°C	.004°C
	pressure	.02	0 to 1500, 0 to 3000, 0 to 6000 dbar	.1% of full scale	.02% of full scale
	salinity	see temp.	30 to 40°/oo	.02°/oo	.003
	sound velocity (optional)	.00007	1400 to 1600 m sec^{-1}	.15 m sec^{-1}	.07 m s
	conductivity	.015	0 to 60 mmhos cm^{-1}	.02 mmhos cm^{-1}	.002 mmhos cm^{-1}
	oxygen	3	0 to 15 ppm	larger of 3%, .15 ppm	.10 ppm

TABLE 2.1 MANUFACTURERS SPECIFICATIONS OF UNDERWATER UNIT (Continued)

INSTRUMENT	PARAMETER	TIME CONSTANT (sec)	RANGE	ACCURACY	PRECISION*
NEIL BROWN MARK III (CTD)	temperature	.03	-3 to 32°C	.005°C	.0005°C
	pressure	not given	0 to 320 0 to 650 0 to 1600 0 to 3200 0 to 6500 dbar	.1% of full scale or .05% of full scale (*optional*)	.0015 %
	conductivity	.03	1 to 65 mmhos cm^{-1}	.005 mmhos cm^{-1}	.001 mmhos cm^{-1}
	oxygen current+ (optional)	1	0 to μ A	2nA	.5nA

* The precision, i.e. repeatability, of the Mark III is limited for some parameters by the quantizing interval, i.e. the digital resolution. The repeatability is larger than the resolution for the 9000 series.

+ Partial pressure of oxygen is a function of oxygen current and sensor temperature.

CTDs. The CTD contains no circuitry to provide salinity. The CTD does contain an additional, fast response, thermister to reduce time lag problems. Its measurements of rapid temperature changes are added to the platinum thermometer measurements before recording. A similar extra sensor is now available as an option on the 9051.

Data is transmitted to the ocean platform continuously by multiplexed, analog, frequency modulated (FM) signals in the 9000 series instruments. A limited frequency band is assigned to each parameter. The multiplexing then allows all parameters to be transmitted simultaneously. At the platform, signal sampling is variable. Temporal resolution is limited by the necessity for a counting interval long enough (~.1 to .3 sec) to distinguish meaningful frequency differences, although techniques of period counting and frequency multiplication exist which can reduce this time by more than an order of magnitude. The Neil Brown CTD first digitizes the sensor outputs every .032 sec and then transmits the data in "TELETYPE" format using frequency-shift-keyed (FSK) modulation. Its temporal resolution is therefore fixed at .032 sec.

Some expansion in the number of parameters measured in a data cycle (or scan) is possible with either system. Besides the dissolved oxygen and sound velocity measurements already available as options, one might expect to see the addition of such parameters as time, pH, nephelometry and water velocity components sometime in the future.

Not mentioned in this treatment are the great variety of shallow water type STDs and CTDs in common use in estuarine and coastal studies. These devices typically are

less precise since they are designed to respond to larger dynamic ranges. Nonetheless, they constitute an important contribution to the STD/CTD archive to be established at NODC.

It must be emphasized that the manufacturers' specifications in Table 2.1 apply for optimal conditions. In general, at sea measurements rarely achieve these standards due to other sources of electronic noise, compromises in the rate of recording data, dynamic errors introduced by differences in sensor response times when passing through high vertical gradients, and sensor drift between calibrations. Not only do these factors degrade data quality from manufacturers' specifications, but they also add to the variability in data quality between separate uses of an identical model. These points are discussed in more detail in following sections.

2.2 DATA LOGGING

The instruments described above are just one part of a data collection system. On board the ocean platform the data are received and are displayed, plotted and/or recorded. During this step the resolution of the logged data can be degraded seriously from the optimum resolution of which the instrument is capable. An analog trace might be produced to give an immediate picture of the stratification. This would be extremely useful in deciding on the course of a cruise, but might depend upon the tedious, and resolution-limited, process of manual digitization for further processing and analysis. In another case the data may be read and stored automatically as they are

plotted but at intervals large compared to the sampling rate in order to save space on a storage device. This method removes much of the tedium and some of the imprecision but discards data that would be useful in reducing both system noise and aliasing by high frequency components. Finally, all the data which the instrument is capable of resolving may be recorded, either in digital or analog form, so that signal processing procedures can be employed to produce data of the highest possible quality at whatever temporal or spatial scale is of interest. Clearly this last is preferable.

All three approaches outlined above are used to obtain the data that will reside in the NODC archive. Early models of digital data loggers (e.g., Plessey, 8114) sampled frequencies in the various bands sequentially and thus the user was not able to avoid data loss. The new models can avoid data loss. The Grundy 8400 Digital Data Logger, an option for use with the 9051 system is an example. It can count cycles over time intervals of .01 to 10 sec according to user needs (but typical intervals are .1 and .3125 sec). The user may specify the number of scans recorded per second so that data loss can be avoided. However, arbitrary selection of these two parameters can still result in data loss. For example, if frequency is determined by counting cycles over a .1 second interval and this is done once each second, 90% of the data are lost.

Even when the selection is done carefully, one must choose between widely spaced points of high precision and closely spaced points of low precision. Resolution is limited by least count error, i.e., the difference between the total, fractional, number of cycles that fit in the interval and the smallest number of whole cycles that might be counted in the same interval. The difference may be

most of a cycle. Thus a resolution of one part in 10^3 requires counting 10^3 cycles, which amounts to most of a second since the STD transmits in the kilohertz range. As mentioned, high precision frequency determinations can be made in shorter times (hence, more closely spaced in the vertical) if period counting or frequency multiplication techniques are used in the data loggers. Period counting uses a crystal clock to generate pulses in the megahertz range that can then be counted to a resolution of one part in 10^3 over the course of a few data cycles. Frequency multiplication scales the transmitted frequency up by one or two orders of magnitude before counting so that 10^3 cycles can be counted in less time. "Home made" data loggers implementing these methods have been built at several institutions for various applications, including the Woods Hole Oceanographic Institution in Massachusetts and the National Institute of Oceanography in Wormley, England.

CTD data are generally operated on by computer to produce digital tapes for subsequent processing. Data logging rates are programmed in and are entirely up to the user. The same care to avoid losing data must be expended.

In summary it is noted that many data loggers, developed in house at some institutions or produced by several different manufacturers, are available. They produce data in many formats. The multitude of formats constitutes only a minor problem because reformatting can usually be performed to produce a tape that can be read at NODC. The most serious problem introduced by the selection of a data logger is that due to discarded data.

2.3 DEPLOYMENT

Most often these instruments are used for vertical profiling. The vertical resolution of the resulting profile depends upon the sampling rate of the data logging device and the rate at which the instrument is lowered through the water (the drop rate). For STDs interpreting FM signals by counting cycles over 0.33 sec, typically, the appropriate sampling rate is 3 times per second. For a reasonable drop rate of one decibar per second, the STD can provide a data point every .33 dbar. Because of dynamic errors in salinities measured by STDs due to temperature sensors lagging conductivity sensors, a 1 dbar sec^{-1} drop rate in regions of rapidly fluctuating gradients usually produces many salinity "spikes" in the record. The user responds by reducing the drop rate to about .3 dbar sec^{-1}. Problems associated with the slower rates (cf. Scarlet, 1975) including ship's roll are more subtle and rarely affect the user's decision on drop rates. A .3 dbar sec^{-1} drop rate provides a point every .10 dbar. (With a .3 sec counting interval and a 3000 dbar sensor, the 9051 data logger can digitally resolve 0.1 dbar, but the sensor noise is .60 dbar and the actual depth may be off by 3.00 dbar). At such drop rates it takes about two hours to profile 2000 dbar. The CTD on the other hand does not compute salinity, so dynamic errors can be eliminated by signal processing procedures at a later step. A CTD will generally be dropped at 1 dbar sec^{-1} and provides a point every .03 dbar, yet still takes just over one half hour to profile 2000 dbar. (For a 3200 dbar sensor the noise is only .04 dbar though the actual pressure may still be in error by 3 dbar, as above).

There is an upper limit on drop rates set by the terminal fall velocity of the instrument. Unwinding

the cable too rapidly may cause loops and kinks to develop that could result in loss of the instrument. Slower drop rates are in order while profiling within a few meters of the ocean floor.

After the device has been lowered to the desired depth it must be returned to the surface, so users often record data (an "uptrace") on the way. The underwater unit is designed with the sensors near the lower extremity so that they lead the entire package through the stratification during lowering. On the return the sensors fall in the wake of the device and thus are deemed capable only of measuring some perturbed version of the actual stratification. Other reasons for using only the downtrace are related to the thermal lag of the massive pressure case of the instrument. Early instruments were apparently designed with the usual warm to cold stratification in mind and thermal effects on the internal electronics assumed the instrument was warmer than the water it was trying to measure.

Most users do not profile to the sea floor of the deep ocean basins. Their primary concern for high vertical resolution lies in the main and seasonal thermocline of the upper one or two thousand meters, or the shallow coastal regions. This is reflected in the choice of pressure sensor ranges as, for example, listed in Table 2.2 for the purchasers of the Neil Brown CTDs.

Some applications of the high vertical resolution measurements call for a time series of vertical profiles. In this use the instrument is raised and lowered ("yo-yoed") to some shallow depth in rapid succession. These profiles can be treated as separate casts for inclusion in a

TABLE 2.2

Neil Brown Instrument Systems, Inc.
Pressure transducer survey, 1976 - 1979

PSI	Decibars	% of Units Sold
300	206	2
500	344	9
1000	689	2
1500	1034	10
2200	1516	23
4400	3033	15
8850	6102	39
		100

Source: G. K. Morrison, NBIS, personal communication

stratification archive such as is planned here. Other applications, such as horizontal profiles (tows) require time or distance as an independent variable and are consequently quite distinct from vertically profiled data.

2.4 CALIBRATION DATA

Components of the various circuitry in these instruments change electrical and/or physical properties to some degree with use, especially under taxing operating conditions. Consequently, the accuracy quoted at the time of purchase may decrease during operation. Periodic recalibration is required. This is usually done in precise environmental tanks either at the user's own facility or by the manufacturer. In either case, the date and results of such a calibration for each sensor in use during a cruise, is a matter of interest.

Calibration shifts are often not uniform drifts between calibration points. At the very least, shipping the instrument to the ocean platform can be hazardous to its calibration. Thus interim standardizations are also required in the form of comparisons to "classical" oceanographic measurement procedures such as water bottle samples with deep sea reversing thermometers for salinity, temperature and pressure. This data is usually acquired by performing traditional Nansen casts at or near the STD/CTD station, or by placing water bottles on the very cable that connects the electronic instrument, or, finally, by placing water bottles, that can be triggered by command from the ocean platform, directly on the instrument (e.g, a Rossette sampler). This last method enjoys the advantage of minimizing the spatial and temporal separation between the STD/CTD measurement and the standardization point. However,

it requires that the instrument come to rest for a few minutes to allow the thermometers to equilibrate. To avoid bottle breakage or sample contamination caused when closed water bottles are brought through increasing pressures, these data are often taken only during the uptrace. This creates the problem of standardizing the downtrace with data from the uptrace.

Another method that has been used does not depend upon nearly simultaneous classical measurements. It uses the fact that historical T, S relations in particular deep water masses are extremely stable and well defined. The validity of the temperature measurement and the steady state of the deep water is implicitly assumed. The results of any of these comparisons that are available are of interest to anyone using the data.

Ancillary measurements made on the water samples such as dissolved oxygen concentration, pH, dissolved silicates and other dissolved nutrients constitute a data set that can be carried along with the calibration data for a more complete archive at NODC.

2.5 NUMBER OF STATIONS

A characteristic of the data collection that must be of concern to the data archival at NODC is the quantity of data that exists and that may be expected over the next years. An order of magnitude estimate is presented here.

Assume the number of STD units in service has increased by 15 units per year over the last ten years. Although STDs have actually been in use over 15 years, the

lower time figure was made to take into account that the probably increased slowly at first. Assume further, that each unit profiles 200 stations per year. The number of stations in existence should be about 150,000.

For the CTD, assume 100 units are now in service and that this number has been reached by an increase of 20 units per year over the last 5 years. Assume that each CTD unit is involved in 400 stations per year. The stations already in existence should number 100,000.

If present rates of growth continue over the next 5 years the total number of new stations taken would be 540,000 which must be added to the already existing 250,000. Thus the number of stations could triple in the next 5 years.

Section 3
SUMMARY OF PROCESSING TECHNIQUES

This section describes ways in which raw data obtained from STDs and CTDs have been processed to final form. As with the previous section, this is an historical approach. Once again the reader is cautioned not to interpret this account as a step by step instruction manual in the processing of STD/CTD data.

3.1 EDITING

Spurious values are often contained in the raw data. They are caused by such problems as kincked conducting cables, occasional computer bit failures, transient electrical power surges, dirty or corroded slip rings and other such common phenomena. To the extent that the spurious values are random, they can often be distinguished from the uncontaminated data which generally fall within definable relationships and constraints. The spurious data can be immediately rejected as unrealistic.

The editing process discovers and deletes the spurious points and can be performed in a number of ways. Historically, for the traces that were manually digitized, editing was done by eye as the operator omitted the spikes. Some of this type of processing probably still occurs. For digital records, data can be tested for values that fall outside absolute limits defined for each sensor. Data can also be tested for differences between successive observations that exceed a defined maximum allowable value for each sensor. Additionally, points may be deleted if they

are several standard deviations from a norm. There is one class of spurious value that occurs in the salinity trace called a "transient" or "salinity spike" which is not random in nature but is caused by the difference in time constants of the temperature and conductivity sensors. This source of error can often be modeled to provide a better estimate of the real values. This process is discussed in a later subsection.

By whatever process, data from STDs and CTDs should be edited by the primary investigator who is in the best position to know which tests for spurious values are appropriate. His procedures should be documented and submitted with the data to NODC.

3.2 SMOOTHING

The signals produced by the sensors always include random noise at levels indicated by the manufacturor. Noise can also be introduced at any step up to and including the recording process. Noisy profiles can not be improved by editing because the levels involved usually are small enough to keep the measurements realistic by both absolute range and maximum difference criteria. In addition, given enough samples, the measurements contaminated by noise can give information about the mean and, with an estimate of the noise level, possibly the variance of the actual profile. The averaging of several points along a limited portion of the profile or other techniques that smooth the profile (i. e., decrease the contribution of high wavenumber components to the profile) constitute an important step in processing the data.

Some degree of smoothing is likely to be performed for most profiles from STDs and CTDs, but the effects of the smoothing can not always be quantified. The manually digitized trace is smoothed by an intuitive process that differs from one person to the next and, probably to a lesser degree, from one pass to another by the same person. In these cases, neither the number of points averaged nor the high frequencies (or wavenumbers) filtered out of the record can be specified. The noise is reduced by this method but to an unquantified degree. On the other hand, recorded data can be smoothed or filtered by algorithms with precisely known properties. Smoothing should be performed after salinity spikes and other deterministic errors have been removed, as discussed in the following sections. However, this is not always done.

The process selected is of interest to those who use the data as secondary investigators. For example, if a profile is to be analyzed in vertical wavenumber space, the spectral characteristics of the running mean applied during data reduction must be known.

3.3 TIME LAG CORRECTIONS

The sensors on these instruments do not respond perfectly to environmental changes. The response of a sensor is often well modeled by an exponential decay function. The decay constant, or time constant, of this function is a measure of how quickly the sensor responds to an impulsive change in the environment. The time constants for any two sensors are likely to be different and the difference in time constant between the conductivity and temperature sensors controls both the accuracy and the precision of the salinity calculated from them. The exponential decay model allows one to correct for much of the difference

but temperature and conductivity time series data are required. They are not available from the 9006 or the 9040.

3.3.1 Salinity Reporting Instruments

If conductivity time series are not available, salinity spikes that occur at depths of sharp changes in vertical temperature gradient can often be removed by an editing process as described in Section 3.1. However, sustained salinity offsets in depth intervals of large sustained temperature gradients can not be corrected in this way. The STD manufacturer does supply an algorithm to estimate this offset (Hytech, 1967):

$$S_e = .35\ (M \cdot V \cdot S \cdot \alpha) \tag{3.1}$$

where S_e = salinity offset ($^o/oo$)

M = sea water vertical temperature gradient ($^oC\ dbar^{-1}$)

V = drop rate ($dbar\ sec^{-1}$)

.35 = time constant of platinum thermometers in temperature compensation circuit (sec)

α = temperature coefficient of conductivity (G) of sea water (G/G per ^oC)

S = salinity ($^o/oo$)

At 5^oC, $S \cdot \alpha$ is equal to one and varies slightly at other temperatures. The use of such procedures has been very common, especially among early STD processors. The use of such a correction during processing of a data set supplied to NODC is an item of interest to the secondary users.

The manufacturer provided sensor time constant of .35 sec may not be effective for the data collection system as a whole and an independent estimate of the effective time lag (i.e., time constant difference between temperature and conductivity sensors) may be necessary. Dantzler (1974) calculates that for certain simplified, but not unreasonable, conditions, the time constant difference can be determined by the salinity offset observed between a rapidly and a slowly lowered STD.

$$S_e \approx \overline{S(t)}_{fast} - \overline{S(t)}_{slow} = \left(\frac{\partial S}{\partial T}\right)_C \left(\frac{\partial T}{\partial t}\right) \tau \qquad (3.2)$$

where S(t) is the time series of salinity

T is temperature (^oC)
t is time (sec)
τ is the time lag = conductivity time constant-temperature time constant (sec).

overbar denotes time average

$\frac{\partial S}{\partial T}_C$ = the dependence of salinity on temperature for a fixed conductivity (o/oo $^oC^{-1}$).

= $\alpha \cdot S$ in equation 3.1

The conditions assumed are that averaging is performed over periods long compared to the effective response times and yet short enough that the variance about a constant value of the actual salinity time series is negligible compared to the offset due to the time lag. For .5 sec sampling in the thermocline of the western Atlantic, he

finds 7 sec an appropriate averaging period. He then finds an effective time lag of magnitude .6 sec.

Dantzler calls this procedure a dynamic salinity calibration, and warns that salinity spikes must not be edited before performing the averaging. While this procedure greatly enhances the accuracy of the salinity record, the smoothing is rather severe. For the lowering rate of his data (1.17 dbar sec^{-1}), 7 sec averaging provides a vertical resolution of only 8.2 dbar. Whether such a dynamic calibration has been performed should be indicated to subsequent users.

For temperature and salinity data in time series and for small time constants, much greater vertical resolution can be maintained using a method outlined by Scarlet (1975). He calculated $\frac{\partial T}{\partial t}$ (as in equation 3.2 and as approximated in equation 3.1 by the product M·V) over the time of just a few scans. For scans separated by a time interval of δ, $\frac{\partial T}{\partial t}$ is determined by an average over N points ($N \geq 1$) and is given by:

$$\frac{\partial T}{\partial t} = \frac{1}{2N\delta}\left\{T\left[(n+N-1)\delta\right] + T\left[(n+N)\delta\right] - T\left[(n-1)\delta\right] - T\left[(n)\delta\right]\right\} \quad (3.3)$$

and is appropriate at the $(n+\frac{N-1}{2})$ th scan. Scarlet (1975) uses N=1 for time constants shorter than several δ. He gives

$$\frac{\partial S}{\partial T_C} = \frac{-S}{0.9}\,(0.028-0.00032\,T)$$

and then calculates the salinity correction using the right hand side of equation 3.2. For noisy data or data

with time constants larger than several scans, he suggests a least squares slope approximation to $\frac{\partial T}{\partial t}$. This procedure should be used on data whose salinity spikes have not been removed. Then the value for τ can be adjusted until the spikes are minimized. This estimate of τ does not then require the large averaging, nor the rapid and slow drops, needed for Dantzler's (1974) method. Scarlet is able to maintain 2 dbar vertical resolution, and finds an effective τ of .16 sec for the 9040 STD. The form of $\frac{\partial T}{\partial t}$, the value of N, and the estimate of τ should be indicated if Scarlet's (1975) method is used to correct time lags of STD data.

3.3.2 Conductivity Reporting Instruments

Conductivity is available from the CTD and from the 9051. It is available from the 9051 in time series form if the data logger uses a counting interval long enough to allow a data record and record gap to be written on tape. Otherwise scans are lost. The CTD data logging program must also be fast enough to prevent lost scans. Then a response correction model, such as described below can be applied.

The treatment summarized here is from Fofonoff et al. (1974). The time response of the temperature probe is assumed to be of the form

$$\frac{dT}{dt} = \frac{1}{\tau}(T_o - T) \qquad (3.4)$$

where T is the measured temperature, T_o is the true temperature at the time of the conductivity measurement and τ is the time lag.

The equation can be solved for the true temperature at the time of the conductivity measurement,

$$T_o = T + \tau \frac{dT}{dt} \tag{3.5}$$

and some improvement can be obtained in the response of the temperature sensor. Estimates of $\frac{\partial T}{\partial t}$ from first differences tend to be noisy, so the profile is first smoothed over N points (cf. Scarlet, 1975) before calculating the time derivative used in equation 3.5. The value for τ is the effective response time of the temperature sensor and circuitry compared to that of the conductivity cell and circuitry. As such, the manufacturer's estimate of time response of the sensor may not be appropriate. In practice the parameters N and τ are selected to minimize salinity spiking. The time corrected temperature is then used with the conductivity measurement to calculate a clean salinity profile.

This algorithm improves the accuracy of the temperature record. However, it decreases the signal to noise ratio of the overall record due to its amplification of the noise-dominated, high frequency end of the measurement band. The signal to noise ratio can be improved by applying a low pass filter after the time lag correction (Fofonoff et al., 1974).

For subsequent use of the data it is important to document the time lag correction scheme employed, if

any, the number of points (N) involved in the smoothing, the effective time lag (τ) chosen and any low pass filtering performed following the correction.

For data recorded sequentially rather than simultaneously an extra step interpolating observations to common times should be taken before time lag corrections. Such a scheme is devised by Roden and Irish (1975).

In the above methods, τ is an adjustable parameter (cf. p. 3-7) whose value is set based upon the elimination of salinity spikes in portions of the water column where the vertical temperature gradient undergoes a rapid change. There is some ambiguity in the choice, with several multiples of a scan interval giving seemingly equal amounts of residual spiking. For example, Fofonoff et al., (1974) indicate that time lags of 5, 6 or 7 scans (.16 to .22 sec) give indistinguishably acceptable results. Joyce (1976) develops a relation between the error in an estimate of the time lag and the drift with frequency (or wavenumber, if the drop rate is constant) of the phase between temperature and salinity gradients. He observes less phase drift with a τ of 5 scans (.16 sec) than with 6 (.19 sec) or 7 (.22 sec) scans thereby making 5 scans the best estimate.

With the fast response temperature sensor now on CTDs, the time lag is much smaller (on the order of 1 scan) and the benefit of the more complicated phase drift test is less apparent. However, a problem with the combined temperature signal is that it is not so well described by the exponential decay model used throughout the above discussions

(Millard et al., 1979). The data needs to be treated by a different filter, with empirically determined weights, to get the proper time and frequency responses to describe features as fine as the one meter scale and finer (Horne and Toole, 1980).

3.4 CORRECTION FOR HEATING BY THE CONDUCTIVITY CELL

Even with perfectly matched sensors, salinity spikes can be produced by the heating (cooling) of water within the conductivity cell by the cell head itself. The temperature of the conductivity cell does not respond perfectly to temperature changes in the environment. This produces a transient temperature difference between the cell and the water in the cell. If the cell passes through the water slowly enough, the water in the cell will gain (lose) sufficient heat from (to) the cell to affect the conductivity measurement. Since the temperature sensor is located elsewhere, this temperature change will go unmeasured and the conductivity increase (decrease) will be assigned to an increase (decrease) in salinity. The result will appear as a salinity spike in portions of the water column where the descent (ascent) rate is near zero.

Scarlet (1975) finds such spikes in his STD data. These spikes ought to be removed before any averaging is done with the data (but after time lag corrections have been made). A procedure for removing them is described by Scarlet (1975). He employes a "latch" type filter which passes only increasing pressures. This effectively removes the heating effect but tends to eliminate points necessary to give the proper average lag corrected temperature (Scarlet, 1975). The occurrence and subsequent removal of

such spikes is of interest to the secondary user. Such spikes are less a problem with the CTD which tends to be lowered through the water more rapidly. The smaller conductivity sensor head of the CTD is not an advantage because the water volume enclosed is also much smaller.

3.5 PRESSURE SORT

In general data are not stored as a time series, but a pressure series. Since the instruments actually respond in time ship roll modulates the lowering rate. Rate changes and even reversals may occur in the pressure time series. Some filtering is necessary to produce a pressure series.

One process that is employed is to interpolate to the desired pressure values. The noise of such interpolated values could be quite high if only two points are used. If interpolation is to be done, as many points as possible should be used to reduce noise. For example, ten points above and ten below the value can be used to calculate a least squares line. Both the interpolation scheme and the number of points involved would be of interest for subsequent use of the data. The choices should be made to minimize the loss of data.

Another method is to average all values in a given pressure interval. This does not throw data away but the pressure series produced may not be entirely uniform and the number of points averaged may vary greatly from one interval to the next depending on the drop rates. For data quality to be assessed, both the typical number of points per pressure bin and the range of the numbers would

be of interest. This information is usually not provided with the data. Empty bins are sometimes filled in by linear interpolation between existing bins. If this is done it should be documented and the number of bins that were filled should be indicated. Indicating individual interpolated bins is even more useful.

3.6 CALIBRATION OF TEMPERATURE AND PRESSURE

Results of the laboratory calibration procedures mentioned in Section 2.4 are often implemented by the use of formulas that relate the correction of the sensor measurement to the temperature and/or the pressure under which the observation is made. (Relationships to salinity are rarely large and are usually undesirable). These corrections are usually applied in the processing stage. This information may be of interest to subsequent users of the data.

Between laboratory calibrations, the validity of the formulas can be monitored by comparison to classical measurements, as mentioned. The STD/CTD temperature and pressure can be compared to measurements by protected and unprotected deep sea reversing thermometers. The precision of these devices ($\pm$.01°C and $\pm$5 dbar) is less than the target accuracy of the electronic measurements (e.g., .004°C and 1 dbar) in some applications, but a sufficient number of observations can greatly improve the estimate of a mean correction. If deep sea reversing thermometer precision is all that is required, only a few measurements need be made. There is great variation in the target accuracies for which collectors of the data aim, and this is reflected in the number of standardization measurements they make.

Experience shows, however, that the temperature and pressure sensors are rather stable and usually drift little during the course of a cruise so corrections can then be determined over several stations. In this way the number of available standardization measurements is greater than the number collected during a single station.

Care should be taken when standardizing the temperature sensor to allow for the difference between the 1948 International Practical Temperature Scale (IPTS) and the 1968 IPTS. The two scales differ (e.g., by .003°C at a temperature of 3°C). The difference has been approximated by Fofonoff _et al_., (1974) using a quadratic equation in the range 0 to 30°C.

$$T_{48} = T_{68} + 4.4\mathrm{x}10^{-6}\, T_{68}\,(100 - T_{68})$$

T_{68} is the 1968 IPTS temperature (as measured by the CTD, for example)

T_{48} is the equivalent 1948 IPTS temperature.

The scale in use during calibration procedures should be specified to NODC for both the electronic sensors and the deep sea reversing thermometers, if used. The distinction again becomes important when making use of the salinity algorithms which are based on temperatures calibrated against the 1948 IPTS.

The accuracy of the pressure reported to NODC is greatly affected by a conversion to depth in the processing stage. As has been indicated, the STD and the CTD measure

pressure. Classically, the vertical coordinate has been depth and there is a tendency among many users to convert pressure measurmenets to values of depth. Many different algorithms of differing accuracy are used in the conversion. If depth is used to calibrate the pressure sensor and/or if depth is reported to NODC in lieu of pressure, the algorithm chosen should also be reported.

Neglecting vertical motions, an increment in pressure (dp) is related to an increment in depth (dZ) exactly by the hydrostatic relation

$$dp = g \rho \, dZ \qquad (3.6)$$

where Z = depth in meters (increasing downward)

g = acceleration of gravity (a function of location and depth) ≈ 9.8 m sec^{-2}

ρ = density of water (in general, a function of location and depth) ≈ 1025-1045 kg m^{-3}

p = pressure in nt m^{-2} .

A convenient unit for pressure is the decibar (dbar) which is 10^4 nt m^{-2}. If P is pressure in decibars

$$dP = 10^{-4} dp = 10^{-4} g \rho \, dZ \qquad (3.7)$$

If pressure, P, and the density profile, $\rho(P)$, are measured, the depth Z^* at pressure P^* can be evaluated exactly from the integral:

$$Z^* = \int_0^{Z^*} dZ = \int_0^{P^*} \frac{10^4}{g\rho(P)} dP = \frac{10^4}{g} \int_0^{P^*} \frac{dP}{\rho(P)} \qquad (3.8)$$

According to equation 3.8, depth can not be calculated until the density profile has been evaluated. The calculation must therefore wait for the salinity determination. A value of g must also be specified. Saunders and Fofonoff (1976) indicate the importance of the geographical and depth dependence of g.

The most accurate approximation of Z^* involves writing a general analytical form for $\rho(P)$, valid for the ocean as a whole or a particular area, and integrating this in equation 3.8. In this case the individual salinity profile for a particular station is not required.

A less accurate approximation claims that $\rho(P)$ is a constant, say ρ_o. Then 3.8 reduces to

$$Z^* = \frac{10^4}{g\rho_o} P^* \qquad (3.9)$$

and ρ_o and g, or the proportionality factor, $\frac{10^4}{g\rho_o}$, should be reported to NODC along with the depths. Grundy estimates that a value for the proportionality factor of .9945 m $dbar^{-1}$ is appropriate for the ocean near San Diego, California (W. Haavisto, personal communication). This type of approximation is usually not appropriate for deep casts. An example is illustrated in Figures 3.1a and 3.1b.

Finally, some researchers use depth and pressure interchangeably. This is the simplest but least accurate approximation since it amounts to setting ρ_o equal to a rather unrealistic 1020 kg m^{-3}, and can lead to confusion if the data are reported to NODC as depth. It is especially problematical if pressure has been calibrated against

Figure 3.1 a & b. Plot showing the relation of values of depth to values of pressure in the upper 500 meters and the upper 3,000 meters respectively. Z is the dimensionless number of meters, to reach a given depth. P is the dimensionless number of decibars at the given depth. X is the dimensionless difference. The triangles represent the observed relation between meter values and decibar values for a station in the North Atlantic ocean determined by a numerical integration of the in situ density values according to equation 3.8. The three straight lines represent various linear approximations to the relationship. The lowest line uses a slope quoted in text appropriate for San Diego. The middle line uses a slope appropriate for the upper 500 meters at this particular station. The top line uses a slope fit over 3000 meters. No slope is satisfactory over the entire range.

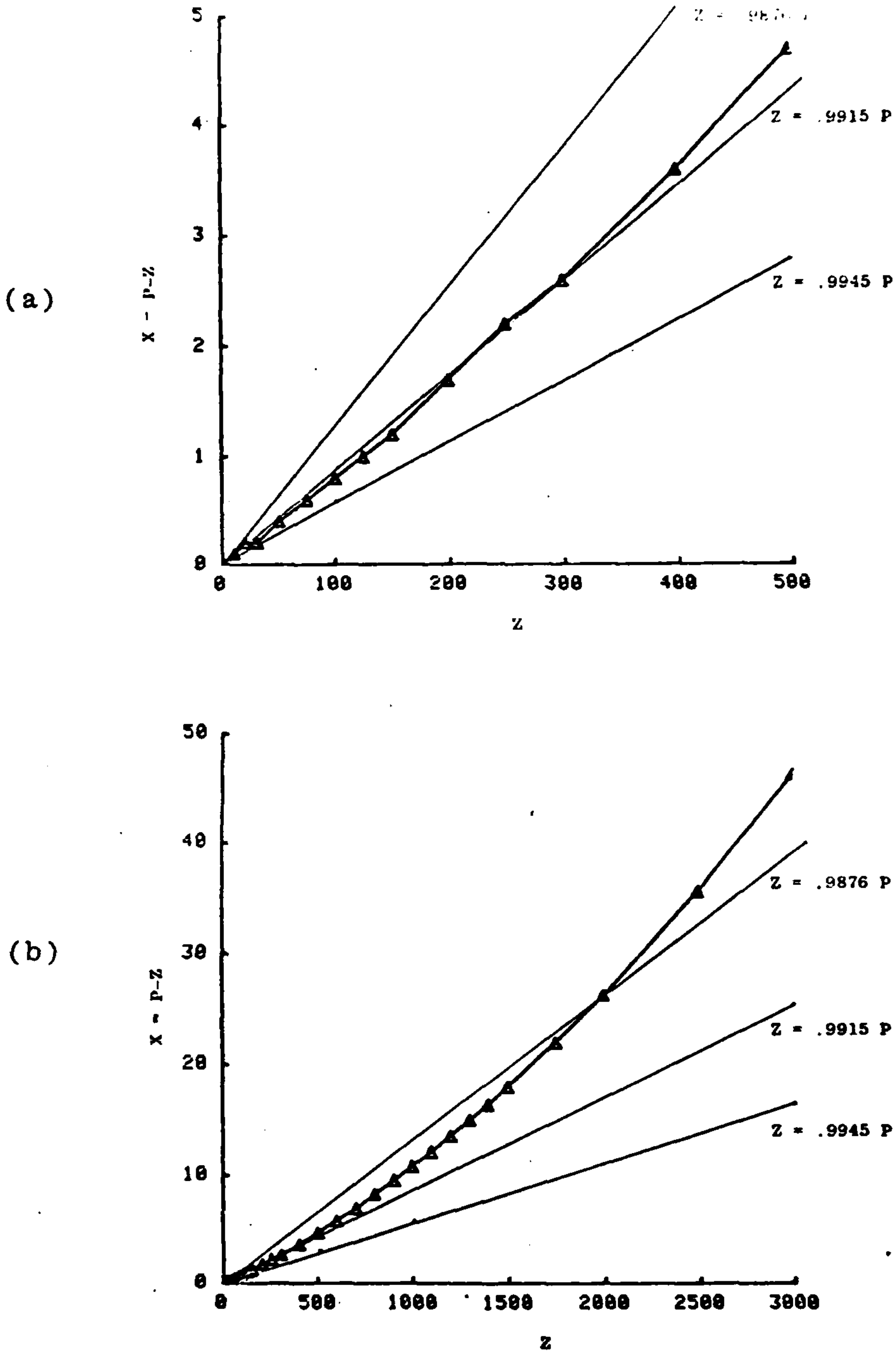

(a)
X - P-Z
Z
Z = .9915 P
Z = .9945 P
0
100
200
300
400
500
1
2
3
4
5
(b)
X = P-Z
Z
Z = .9876 P
Z = .9915 P
Z = .9945 P
0
500
1000
1500
2000
2500
3000
10
20
30
40
50

Figure 3.1

depth in deep water, however, calibrations against depth, rather than other pressure measurements, are rare.

3.7 SALINITY CALCULATION AND CALIBRATION

Conductivity measurements are not calibrated directly during the course of a cruise, due in part, no doubt, to the difficulty of reproducing the pressure and temperature of a water sample once on board. Rather, the derived parameter, salinity (which must be identical for the water sample both *in situ* and on board, regardless of changes in pressure and temperature) is calibrated.

It is most convenient, and completely sufficient, to express a measurement of conductivity (C(S,T,P)) in terms of its ratio (R) to the conductivity of water with a fixed temperature (T_o), salinity (S_o) and pressure (P_o).

$$R = \frac{C(S,T,P)}{C(S_o,T_o,P_o)}$$

The contributions to this ratio can be separated into parts, as done, for example, by Fofonoff *et al*. (1974):

$$R = \frac{C(S,T,P)}{C(S_o,T_o,P_o)} = \frac{C(S,T,P)}{C(S,T,P_o)} \cdot \frac{C(S,T,P_o)}{C(S_o,T,P_o)} \cdot \frac{C(S_o,T,P_o)}{C(S_o,T_o,P_o)}$$

These parts represent the pressure effect (R_P, a function of P, T and S), the salinity effect (R_S, a function of T and S) and the temperature effect (R_T, a function of T only), respectively. The oceanographic literature is the source for the (varied) functional forms of R_T (T), R_S (T,S) and R_P (T, S, P). R is output from a calibrated conductivity sensor, T is available from the temperature sensor(s) and P is available from the pressure transducer. R(T) can then be calculated. R_P depends weakly on salinity and for a guess, S_1, can be calculated also. Then the value R_S can be computed:

$$R_S = \frac{R}{R_T(T) \bullet R_P(T,S,P)}$$

The functional dependence of R_S on T and S can be inverted to give S as a function of T and R_S. Hence

$$S = F(R_S,T) = F\left(\frac{R}{R_T\ R_P},T\right).$$

This value is not correct for it depends upon the initial guess S_1 used in the calculation of R_P. This S (now S_2) can be used in a recalculation of R_P that will give a new value for S (now S_3). This iterative process continues until $|S_{n+1}-S_n|$ is less than some specified tolerence, say .003°/oo. Then S_{n+1} is taken as the salinity (S) of the water.

There are several sources of the formulas for R_P, R_T, and $F(R_S,T)$ mentioned above. Most use reference

values of T_o=15°C, S_o=35°/oo and P_o=0 dbar. Fofonoff et al. (1974) refer to Brown and Allentoft (1966) for $R_T(T)$. Lewis and Perkin (1978) also indicate Thomas et al. (1934) as a source. For R_P (T,S,P), Bradshaw and Schleicher (1965) published the data used when this correction is made although the functional form is sometimes refit. (Note that bench-top salinometers which operate at a gauge pressure of 0 dbar=P_o, do not require this correction.) For R_S and its relation to salinity, the UNESCO tables (UNESCO, 1966) based on the work of Cox et al. (1967) can be used. First a new ratio, $R_{15} = \frac{C(15,\overline{S,0})}{C(15,35,0)}$ is defined and this ratio is given as a function of T and R_S. The salinity is defined as a function of R_{15}. The same procedure is used with different data by Brown and Allentoft (1966) as well as Thomas et al. (1934). A summary of algorithms in use among respondents to a mail survey is given in Table 3.1 reproduced from Lewis and Perkin (1978). Discrepancies are inherent in the varied computations outlined in the Table. Lewis and Perkin (1978) estimate differences up to .02°/oo but perhaps confined to .005°/oo for the newer more reliable, data and fits. The discrepancies arise from different techniques for varying salinity and incomplete coverage of the oceanic ranges.

While users of CSTDs and CTDs have their option in combining algorithms for salinity calculations, the STD consists of hard wired circuits that implement the UNESCO relations for converting R_S and T to R_{15} and then R_{15} to S. The circuits that compensate for pressure and temperature effects (i.e., that model R_P and R_T) are based on

Table 3.1

Data Sources of Equation Sets Used for CTD Measurement Reduction

Equation Set	Number of Users	Information Source: Pressure Correction	Temperature Dependence of 35‰ Water	Correction to Conductivity Ratio (Δ_{15}) *	$R_{15} - S$	Other
Unesco [1966*a*]	8			C (S)	C (S)	
Perkin and Walker [1972]	7	BS (R)	BA (R)	BA (R)	BA (R)	Dauphinee for $T < 1°C$: *Reeburgh* [1965] for $C(35, 0, 0)$
Fofonoff et al. [1974]	6	BS (S)	BA (S)	C (S)	C (S)	
Bennett [1976]	5	BS (R)	BA (R)	C BA (R)	C (S)	Dauphinee for low temperature
Gascard [1970]	1	BS (S)	BA (S)	C (S)	C (S)	*Weyl* [1964] for $C(35, 15, 0)$
Jaeger [1973]	1	BS (S)	BA (R)	BA (S)	BA (S)	
Zaburdaev et al. [1969]	1	BS (S)	BA (R)	C (S)	C (S)	*Weyl* [1964] for $C(35, 15, 0)$
Accerboni and Mosetti [1967]	1		BA (R)	C BA (R)	C BA (R)	
Rohde [1972]	1	BS (R)	T	T	T	
Ribe and Howe [1975]	1	BS (R)	BA (R)	C (R)	C (R)	
Fedorov [1971]	1	BS (R)	BA (R)	C (S)	C (S)	
J. Crease (unpublished data, 1977)	1	BS (R)	BA (R)	BA (unpublished)	C (S)	
Thomas et al. [1934] *Bradshaw and Schleicher* [1965]	1	BS	T (S)	T (S)	T (S)	

BS is *Bradshaw and Schleicher* [1965], BA is *Brown and Allentoft* [1966], C is *Cox et al.* [1967], and T is *Thomas et al.* [1934]. (S) denotes same equation as data source, and (R) refit to data.

Source: Lewis & Perkin, 1978.

* The algorithm referred to here converts R_s & T to R_{15}.

the algorithms of Bradshaw and Schleicher (1965) and Brown and Allentoft (1966), respectively.

The salinity calculations outlined above depend upon a calibrated conductivity ratio measurement. The *in situ* conductivity cell is calibrated by comparison with simultaneously collected water samples whose salinities are determined independently using a bench salinometer. The conductivity cell requires frequent recalibration because of drift in conductivity between stations. The salinity determined from the salinometer is used with the *in situ* measurements of temperature and pressure to calculate a conductivity ratio R. The output of the conductivity sensor (G) is then related to this ratio R by the cell constant (k) of proportionality.

$$R = k \cdot G$$

The cell constant (k) is adjusted to give a proper value of R for each station. Some users select their k to give absolute conductivity rather than the ratio R but this is not necessary. The cell constant changes primarily because of changes in cell geometry which are most often caused by deposition of material (to which the small CTD cell is particularly susceptible) but may also be related to temperature and pressure effects. The temperature and pressure effects on the geometry of the CTD cell have been modeled by Fofonoff *et al*. (1974). The calibration of STDs and CTDs are in practice often expressed in terms of additive salinity offsets (ΔS) rather than shifts in cell constant (k), but such corrections really apply only in the limited ranges of T, S, and P which the water samples span.

The ΔS may also be obtained if a historical θ, S (i.e., potential temperature, salinity), relationship exists which is tight, i.e., for a given θ there is no more uncertainty in S than can be tolerated by the target accuracy, say .003°/oo. For the Western Atlantic, such a relationship has been used in the θ range 2 to 2.5°C which lies at pressures near 4000 dbar (e.g., Worthington and Metcalf, 1961 cited by Fofonoff et al., 1974). However, recent work has shown that anomalies occur within the deep water masses (McCartney et al., 1980).

Once ΔS has been established, the associated ΔC can be determined by the relation (Fofonoff et al., 1974):

$$\Delta C = \Delta S \left.\frac{\partial C}{\partial S}\right)_{T,P,\bar{S}}$$

where $\Delta S = S_{standard} - S_{CTD}$

C = conductivity change

T = CTD temperature, corrected

P = CTD pressure, corrected

$\bar{S} = 1/2\,(S_{CTD} + S_{standard})$

$\left.\frac{\partial C}{\partial S}\right)_{T,P,\bar{S}}$ = dependence of conductivity on salinity for given temperature, salinity and pressure (to the nearest thousandth)

The value of $\frac{\partial C}{\partial S}$ can be tabulated from existing data, or the fit for deep water over most of the worlds oceans, given by Fofonoff et al., can be used

$$\frac{\partial C}{\partial S} = .790 + 2.2\times10^{-2}\,(T-1.0) + 6.9\times10^{-6}\,(P-2400) + 3.75\times10^{-3}\,(35-S).$$

Then ΔC can be used to determine a new cell constant according to the formula

$$k_{NEW} = k_{OLD} \cdot \frac{(C_{CTD} + \Delta C)}{C_{CTD}} .$$

The ratio $(C_{CTD} + \Delta C)/C_{CTD}$ is called the cell factor (C.F.). The old cell constant can be replaced by the new one. Alternatively, the value of K_{OLD} can be held fixed while C.F. is allowed to vary from one station to the next. The values of C.F. will be close to 1.0.

The bench salinometer provides salinity calculated from a conductivity measurement whose conductivity cell is more stable than the _in situ_ cell. The same choice between equations must be made to convert conductivity to salinity. Good agreement, on the order of the instrument noise ($\pm$.003°/oo), can be obtained by modifying the _in situ_ measurements by the simple corrections mentioned. In this manner salinities from stations on the same cruise can be compared down to the noise level (e.g., .003°/oo, Fofonoff _et al_., 1974) and this is the accuracy most researchers claim. However, as mentioned, the formulas relating conductivity to salinity come from a variety of fits to several, incompatible, data sets which leads to computational discrepancies of up to .02°/oo. Thus, in general, salinities measured by different researchers can not be compared at the levels of accuracy claimed by those investigators. For this reason, the specifics of the salinity algorithms used by suppliers of the data for both _in situ_ and bench-top measurements are of interest to NODC.

If the same algorithms are used in the conversion of the bench-top conductivity measurement to salinity that are used in the conversion of the _in situ_ measurement, then the conductivity of the _in situ_ cell has actually been calibrated against the conductivity of Copenhagen waters, even though the salinity has not. Conductivity values can then be used in a recalculation of salinity based on the user's preference or requirements. In addition, as a new practical scale for salinity and density in terms of conductivity of Copenhagen water is in development (Lewis & Perkin, 1978), the calibrated conductivity measurements will be of value when these algorithms are introduced.

Section 4
THE SECONDARY USER COMMUNITY

4.1 USER CATEGORY

Three types of secondary users have been identified. These are: industrial, government and academic. The uses that each of these groups make of the historical data file are quite different. These are discussed briefly below.

4.1.1 Industry

Most industry users require data from the historical file for two purposes. One is for site surveys in compliance with federal regulations for commercial operations. The other is for environmental information for design purposes. The first requirement normally does not demand much accuracy or resolution. Usually temperature and salinities correct to within $\pm$ .5° C and .05 $^{o}/_{oo}$ suffice along with a measure of the natural variability of the region. (These figures come from a review of offshore environmental consultants). Environmental information for design purposes is much more stringent. This often requires site specific surveys to obtain detailed temperature, salinity, and current information. We do not see the NODC historical data base playing a major factor in design studies.

4.1.2 Government

The government agencies most likely to require data from the historical file are the Bureau of Land Management (BLM), the Environmental Protection Agency (EPA), the Department of Energy (DOE), the National Oceanic and Atmospheric Administration (NOAA), and the U.S. Navy. The first four agencies may have requirements similar to those given for the first industrial use. More accurate requirements may also be necessary but these are usually deferred to industrial or academic consultants. These requirements are given in the section on academic users. The Navy sometimes uses the climatological data for construction of sound velocity profiles. This use requires temperature and salinity precisions of about $\pm$ .1^{o} C and $\pm$ .1 ^{o}/oo respectively. Nonacoustic data requirements for the Navy have not yet been established but are likely to be more stringent (on the order of 1 decibar, .01^{o}C and .01^{o}/oo).

4.1.3 Academia

The academic users generally are engaged in some aspect of basic research. Uses of the data may range from input for global numerical models of the ocean circulation and climate, to repeated survey comparisons, to specific process oriented studies.

Often the data accuracy requirements of these studies push the technology available to make the measurements. Because their requirements are the most stringent of all user types and because they traditionally have been

the biggest suppliers as well as users of the NODC data file we have focused on the requirements of the academic community. The study is also restricted to typical usage. Equipment and techniques used in fine structure and internal wave process studies, for example, are not considered.

In order to determine the accuracy and other requirements of the secondary users we elected to conduct an in depth survey of the needs of a few users. The criteria for selection were a reputation for careful work and a history of being either a supplier or user of NODC historical data. The investigators selected represent the most significant ocean climate programs including POLYMODE, CUEA, NORPAX, ISOS and GEOSECS. Taken in total the people contacted in the survey have had experience with the following instruments: Neil Brown CTD, Bisset Berman STD, Geodyne CTD, and both Plessy STD's and CTD's.

Broadly speaking three topics were explored with each of these investigators. The first topic covered their requirements as to accuracy and resolution of NODC data. This topic is the subject of Section 4.2. The second topic dealt with the importance of documenting procedures employed in obtaining the data. This subject is discussed in Section 4.3. Finally, the subject of NODC's involvement is discussed in Section 4.4.

4.2 DATA REQUIREMENTS

The investigators consulted had a wide range of applications for data they might request from NODC. It is not surprising then that their data requirements also varied.

A first issue dealt with the data that should be available on file. In addition to temperature and pressure the data file should include conductivity and salinity or the algorithm connecting these. If oxygen and nutrients are available these would also be useful. Less interest was expressed in observed sound velocity although there was no objection to maintaining this file if it didn't replace the other variables.

The next issue, the pressure interval for which they desired temperature and salinity data, sparked considerably more varied opinions. The most stringent requirement was that for data every decibar, although this was needed only in the upper layer. The least stringent requirement was that for data at standard levels (see Table 4.1). Most other investigators felt that 2 dbar intervals were quite sufficient for their requirements.

At this juncture we consider the philosophical basis for a 2 dbar historical stratification data file. The purpose of such a file is to record the characteristics of the water column at the time and place of the station. The station does not occupy an infinitesimal point but occurs over an interval of a few hours, during which time the ship may drift several kilometers. Ocean processes that occur on smaller time and space scales than this require special procedures and process-oriented studies. Their effects are not adequately described by a historical stratification data set. Natural variability on these scales are caused by ship roll, internal waves and by fine and microstructure.

Table 4.1

34 NODC Standard Depths
(meters)

0	900
10	1000
20	1100
30	1200
50	1300
75	1400
100	1500
125	1750
150	2000
200	2500
250	3000
300	4000
400	5000
500	6000
600	7000
700	8000
800	9000

Source: National Oceanographic Data Center, 1974.

Typical horizontal coherence lengths for fine structure in the upper ocean are of the same order as ship drift distances (Katz, 1973). Below the main thermocline the horizontal coherence lengths are usually much larger than the ship drift.

Ship roll may be a more serious problem. In extreme cases it may have a range of 5 meters. A more typical upper bound on the vertical variation produced by this effect is 2.5 dbar. This is well within the resolution of modern STDs and CTDs.

The internal wave field is also a source of variability. Of most concern are oscillations near the Brunt Väisälä frequency. As the waves near this frequency are very nearly horizontally polarized, the particle motion is nearly vertical. Typical frequencies are 5×10^{-4} sec^{-1} which have periods very near the station time. The vertical displacements at these frequencies could be of the order of 10 meters in the thermocline. Outside the thermocline region, the displacements are considerably less. In the deep ocean the internal wave motions are also highly coherent with depth. It is not likely that the effect of internal waves on the perceived vertical stratification there will exceed 2 dbar.

Finally we consider the vertical scale of transient temperature and salinity structures in the vertical profile. Because of mixing, small scale vertical features may only exist for a few hours, the lifetime of a

station. A characteristic vertical scale for the short lived fine and microstructure appears to be 2 dbar or less (Muller, et al., 1978).

Thus for a historical stratification data file, a vertical resolution much finer than 2 dbar (4 dbar vertical wavelength) does not seem warranted even when an instrument is capable of it.

It is clear from our discussions that data is desired at much finer intervals for the upper ocean than below the thermocline. The discussions explored a number of possibilities for defining this more precisely but none seemed universally applicable. In the absence of such a definition it is considered appropriate to maintain the high resolution throughout the water column.

For some users, station data with much degraded vertical resolution are adequate. The procedure for generating the degraded profiles must be chosen with care. While the standard levels listed in Table 4.1 are useful for many purposes, an expanded set of standard levels would be even more useful. For the accurate determination of geopotential anomaly, observations should not be spaced farther apart than 200 dbars (J. Reid, personal communication). A possible set of expanded standard levels is presented in Table 4.2 modified from a suggestion by A. Amos (personal communication).

Even an extended set of standard levels do not necessarily describe some aspects of the profile that are of

Table 4.2

101 EXTENDED STANDARD LEVELS (meters)

Increment:	2	5	10	20	25	50	100	200	200
	0	35	60	120	225	550	1100	2200	6200
	2	40	70	140	250	600	1200	2400	6400
	4	45	80	160	275	650	1300	2600	6600
	6	50	90	180	300	700	1400	2800	6800
	8		100	200	325	750	1500	3000	7000
	10				350	800	1600	3200	7200
	12				375	850	1700	3400	7400
	14				400	900	1800	3600	7600
	16				425	950	1900	3800	7800
	18				450	1000	2000	4000	8000
	20				475			4200	8200
	22				500			4400	8400
	24							4600	8600
	26							4800	8800
	28							5000	9000
	30							5200	9200
								5400	9400
								5600	9600
								5800	9800
								6000	

interest, specifically, isothermal and isohaline layers. These characteristics are considered in a technique of data compression proposed by the International Council for the Exploration of the Seas (ICES). That scheme requires that data be recorded at the 34 standard levels and at flexture points, spaced such that linear interpolations will not deviate more than 0.03° C and 0.04°/oo from the original record. NODC's experience shows that 110 to 130 levels are selected from a typical STD/CTD station using this scheme (P. Hadsell, NODC, personal communication). The ICES recommendations allow the criteria to be relaxed until the number of points retained is less than 100.

Other schemes to degrade the resolution of a STD/CTD profile involve least squares techniques. These techniques essentially filter out the high wavenumber components to the record. However, the resulting smoothed profiles in general produce T,P, T,S, and S,P points that are not observed in the original profile.

4.3 DOCUMENTATION REQUIREMENTS

On the subject of background information, all those questioned felt the type of instrument and drop rate should be available for each set. In addition, interest was expressed by some in the data logger used and the digitization procedures. Processing steps such as editing, time lag correction, smoothing, production of pressure series and the salinity algorithm were also mentioned. The calibration procedure was mentioned too. It was pointed out that the bottle data would be useful as a calibration check but only if it were from deep waters.

As to quotes of data quality, most investigators' reactions were to accept the data at face value unless interpretation problems arose. In this case the investigators felt it would be best to contact the data supplier directly. Therefore, the institution and investigator supplying the data should be available to the secondary user. The scientific emphasis of the cruise was also of interest.

4.4 REQUIREMENTS FOR NODC ACTION

Opinions were solicited on what actions NODC might take. One question investigated was what tests, if any, should NODC perform on the data submitted. Most investigators felt that it was generally appropriate for NODC to test the data but other than comparisons with climatology no specific suggestions were made.

None though it was appropriate for NODC to perform any noise level suppression. This was regarded as an unnecessary explense which could result in a possible loss of data. It was felt that noise suppression was the responsibility of the data supplier.

The question of which data product options NODC should support for secondary users was also explored. All favored data as submitted. There was little enthusiasm for raw data (either as submitted or as processed by NODC). As to calculated variables, a few felt it might be appropriate for NODC to supply calculated values of sound velocity, Brunt Väisälä and σ_θ but that NODC should charge extra for this extra service.

The investigators were also asked whether it was appropriate for NODC to recommend a format for submitted data. Most felt that a recommended format would be desirable as long as there was some flexibility. It was felt that if a format were recommended it should not be changed without good reason.

Finally, the question was addressed whether NODC should recommend procedures for the collection and processing of STD/CTD data. Some users felt that it was appropriate for NODC to recommend general processing guidelines but that it was inappropriate to require specific averaging techniques. In any case, care must be exercised to avoid directing a description of processing procedures toward a few select instruments (and manufacturers).

Section 5
TESTING DATA QUALITY

Given the wide range of factors influencing the quality of the data, how can data quality be assessed? As the group responsible for STD/CTD data quality control, the Data Processing Branch of the Data Preparation Division of NODC needs this question addressed. The details of several candidate quality control checks are outlined in this chapter. They are not mutually exclusive, but they require ever increasing expenditures of computational resources, and therefore, may not all be possible to implement at NODC. It is assumed here that the data supplied to NODC is in the form of a pressure series and not a time series. Therefore, recalculation of time lag corrections and temperature conductivity coherences are not possible.

5.1 SCALE OF INSTRUMENTAL STRUCTURES

Pingree (1971) described the interaction of time lag between the temperature and <u>pressure</u> sensors. He found regularly spaced features could be produced in an STD trace of a uniform gradient in the presence of ship roll. The depth scale of these instrumental features is given by the product of the drop rate and the period of the ship roll. Observations of period of ship roll are rarely reported with the data so this test can not be of general use, unless some increased effort to observe and report the roll period is undertaken by the oceanographic community. When possible the scale depth should be identified and reported so that it may be taken as a warning by those who would use the data.

5.2 CALIBRATION CHECK

It is possible to use water bottle measurements supplied with the STD/CTD data to check the calibration of the latter data. The check should not be made in the upper layers of the ocean unless the water sampling device is close to the electronic sensors and is tripped during the same trace (down or up) as the electronic data reported to NODC. Sample closeness could be defined in terms of the target accuracy and vertical gradient. For example, if the target accuracy for temperature is .01°C and the vertical gradient is .003°C $dbar^{-1}$, then the reversing thermometer must be closer to the STD/CTD than 3.3 dbar. The surface mixed layer may often allow such a comparison to be made (Amos, personal communication). The definition of upper layers would have to depend upon some local historical perspective unless some arbitrary, but conservative, pressure were selected, say 3000 dbar.

Because of noise in the measurements by both the electronic and classical techniques, a bias in the STD/CTD data can not be determined by just one or two comparisons. The proper method for determining the bias requires generating a histogram of the differences between the STD/CTD and classical measurements. Recall, only measurements of the same water type are being compared because of constraints imposed on closeness of the measurements. For a properly calibrated instrument, the histogram should be symmetric about a peak value of zero difference with a variance that is a function of the noise levels of both techniques. A bias, i.e., calibration error, would then be indicated by a histogram with a peak value at some

non zero difference greater in magnitude than the confidence interval about the mean of the distribution. A 95% confidence interval is appropriate. The size of the 95% confidence interval depends upon the variance of the histogram and the number of comparisons included in it. Assuming a normal distribution for the histogram a confidence interval can be calculated using Student's t distribution. Let X be the mean value of the histogram and s be the square root of the histogram variance. Then the 95% confidence interval on the mean is $X \pm \Delta X_{.95}$ where

$$\Delta X_{.95} = t_{n-1}(.975) \frac{s}{\sqrt{n}} \tag{5.1}$$

where n = number of samples and $t_{n-1}(.975)$ is the appropriate value of Student's function. To be able to determine a bias as small as the variance of the histogram (s) requires that $\Delta X_{.95} \leq s$, which implies $n \geq 7$. To determine a bias as small as half the root of the variance requires $n \geq 20$. To reduce the bias to one tenth of the root of the variance requires 400 comparisons. Often comparisons are made over several stations. These can be combined in a valid determination of the bias only if the bias is nearly constant over that interval of time.

The variance of the histogram is due to the measurement noise of the classical as well as the electronic techniques, as mentioned, but in general the noise of the classical measurements is much greater. Enough electronic measurements are generally available so that averaging can be employed to keep its noise negligible. Thus s is about

equal to the rms noise in the classical measurement. After comparison to 7 water bottle measurements, the possible bias in the electronic measurements is about the same as the error in the classical measurements, but whereas the noise of the classical measurements can be reduced by averaging several together, the bias in the electronic measurements can not be reduced by averaging. Only more comparisons with water bottles can reduce the bias.

Any specified accuracy can be achieved either by making enough comparisons or by reducing the variance of the comparisons (s^2). The variance can be reduced by using a less noisy standard (in effect, the route taken during a laboratory calibration). The value of salinity (S) for a particular potential temperature (θ) in the deep ocean might be a less noisy standard than water bottles (Fofonoff et al., 1974). To produce such θ, S relationships requires the careful analysis of highly reliable data. So far this has been done only in limited regions. To be useful as a calibration check, deep water θ, S relations must be determined for every ocean basin. The source for the deep waters are in the high latitudes so in those regions the θ, S relationships are more variable and less suitable as standards. Comparisons to θ, S standards have the advantage over direct water bottle comparisons of providing more comparisons (e.g., data averaged every .05°C for half a degree for each station) each with a lower variance. In addition, the standard is common to all cruises in the area so no assumptions need be made about the accuracy of water samples supplied with the data. Unfortunately, the

procedure will inhibit the observation of any long term, secular trends that may exist in the characteristics of deep waters. Finally, there are indications that enough variability exists in the deep waters to prevent an accurate comparison (McDowell and Rossby, 1978 and McCartney et al., 1980).

Although substantial effort is required to produce θ, S curves for most deep areas, the effort need be made just once. The environmental models extant at NODC (D. Hamilton, personal communication) are not appropriate for a calibration check. In those models observations are grouped in a kind of volumetric analysis. The salinity bin width is 0.1°/oo, one to two orders of magnitude too coarse to be useful for calibrating STDs and CTDs in deep water. In addition, the choice of ordinates, salinity vs. density (σ_t units), is awkward for the procedure described above. Salinity vs temperature would be more accurate and simpler to use.

5.3 STABILITY CHECK

The ocean is stably stratified. Although processes do work in the ocean to change the density of a water parcel, any resulting stratification with high density overlying lower density water is rapidly corrected by convective overturning and further mixing. In most cases, the observation of lower density at greater depth indicates faulty measurement(s). Usually the instability is eliminated upon removal of a single measurement. The requirement for stability constitutes a powerful quality control test.

In situ density varies predominantly with pressure. If the first of two water types were less dense than the

second at the same pressure, but instead occurs at a greater depth, the greater pressure could give it an *in situ* density greater than that of the second water type. This is less a problem with closely spaced observations or shallow casts, but nonetheless indicates that *in situ* density is not the density of interest. An instability exists if the shallower of two water types is denser than the deeper when both are brought to the same pressure. The density of a water type at an arbitrary reference pressure, independent of its *in situ* pressure, is its potential density. Adiabatic corrections to the temperature must be made during the calculation of potential density.

For comparing the density of water types at two different pressures, the choice is not arbitrary. The pressure effect on cold water is more pronounced than on warmer waters. Cold fresh water that is less dense than warm salty water at a pressure of 0 dbar, may be denser at a pressure of 4000 dbar. Such a situation occurs, for example, in the Atlantic Ocean where Antarctic Bottom Water underlies North Atlantic Deep Water. *In situ* that water column is stable, but it would be unstable at 0 dbar. In order that a quality control test not fail realistic measurements the reference pressure must vary as a function of the pressure of the observations. One workable function is a reference pressure of 500 dbar for observations in the upper 1000 dbar, a reference pressure of 2000 dbar for observations between 1000 and 3000 dbar, and a reference pressure of 4000 dbar for deeper observations. For essentially the same computational expense, adjacent observations can be compared at an intermediate pressure that would vary with every pain of observations.

Any observation leading to an instability can either be deleted or labeled as suspicious. Since

instabilities can exist for short times in the ocean, measurements of such real, albeit transient, phenomena would be sacrificed if removal were uniformly applied. Labeling would enable rapid location of suspicious data by the secondary user while leaving the analysis required before removal up to him. However, labeling increases the information which must be carried along. In either case, the number of instabilities discovered in the station would be kept to indicate problem stations.

Each point in an STD/CTD profile is, in general, the average of several measurements. A spurious instability larger than the noise level of the instrument implies serious problems. Either a few very bad, random, points have not been properly edited, or the assumed precision of the measurements is incorrect. If the occurance of instabilities can be correlated to the layers of high temperature gradient, residual time lag problems may be the cause of the lost precision (R. Millard, personal communication). The correlation would then be high where the temperature gradient change were large.

5.4 NOISE LEVEL TEST

The information concerning the instrument and the deployment, logging and processing procedures can be made available to the secondary user. However, although all this information gives some indication of the data quality, a quantitative measure of that quality, whether it be a ranking or a quoted noise level and/or vertical resolution, is probably not attainable from this information alone.

Fortunately, the data itself can sometimes be tested for these measures of quality following a procedure sketched by Fofonoff et al., (1974). Pressure sorted data, with linear trends removed by first differencing, are Fourier analyzed to produce vertical wavenumber spectra.

In the wavenumber bands in which the oceanographic signal is dominant, the spectral density decreases with wavenumber. At high wavenumbers the spectra flatten as white noise begins to dominate. A wavenumber can be selected at which the sloping part intersects the flat part. Here the signal to noise ratio is one. The associated vertical wavelength can then be taken as the vertical resolution of the data -- regardless of the vertical spacing provided by the originator of the data.

In addition, assuming white noise throughout the measurement band, the spectral level at the noise dominated wavenumbers can be extrapolated through the entire spectrum to estimate the variance of the noise for the parameter being plotted.

Of course, the test only works if data are reported more densly in the vertical than the wavenumber at which the spectrum flattens. Otherwise the spectral level decreases to the Nyquist wavenumber, and all that can be claimed is that down to the reported vertical resolution the signal dominates the noise. Estimates of the variance of the noise then can not be made.

The noise level and vertical resolution will likely be different in portions of the water column with different gradients (as was found by Fofonoff et al., 1974). However, for the simple quality indicator desired here a single test of the noise level for the entire station can be considered sufficient. The noise level should be reported with the station for the benefit of the secondary user who can decide for himself whether and how to filter the data.

The spectral analysis outlined above is likely to be very demanding on computational resources. It may prove impractical to apply the test for each station in NODC's possession. The technique is still of use, as a spot check performed a few times for each cruise of data. The results can be reported for every station on the cruise in the latter case.

Section 6
RECOMMENDATIONS

It is considered that NODC's duties would be satisfactorily executed by implementing the system outlined in block form in Figure 6.1. A discussion follows here. More specific descriptions are to be contained in a companion report (Molinelli and Stieglitz, 1980).

6.1 DOCUMENTATION

Presently, NODC requests information on STD/CTD data it receives on a Data Documentation Form. In light of the information required regarding the collection and processing of STD/CTD data summarized in Chapters 2 and 3, it is recommended that the Data Documentation Form, especially Part B. Scientific Content, be revised. It should ask specifically about the procedures indicated in those chapters. The present version is reproduced in Appendix A. The recommended revision is given in Appendix B. The purpose of this documentation is not to allow NODC or the secondary user to reprocess the data, but instead to let the secondary user know if those steps he considers critical for his applications have been performed on the data. The paper form presented in Appendix B need not be used if data is exchanged in the fixed format described below. In that format the information in Appendix B is entered as computer character text on the exchange tape.

6.2 EXCHANGE

Inherent in the vast number of data points characteristic of STDs and CTDs is the need for computerized processing, storage and exchange. During exchange, data

STD/CTD DATA FLOW AT NODC

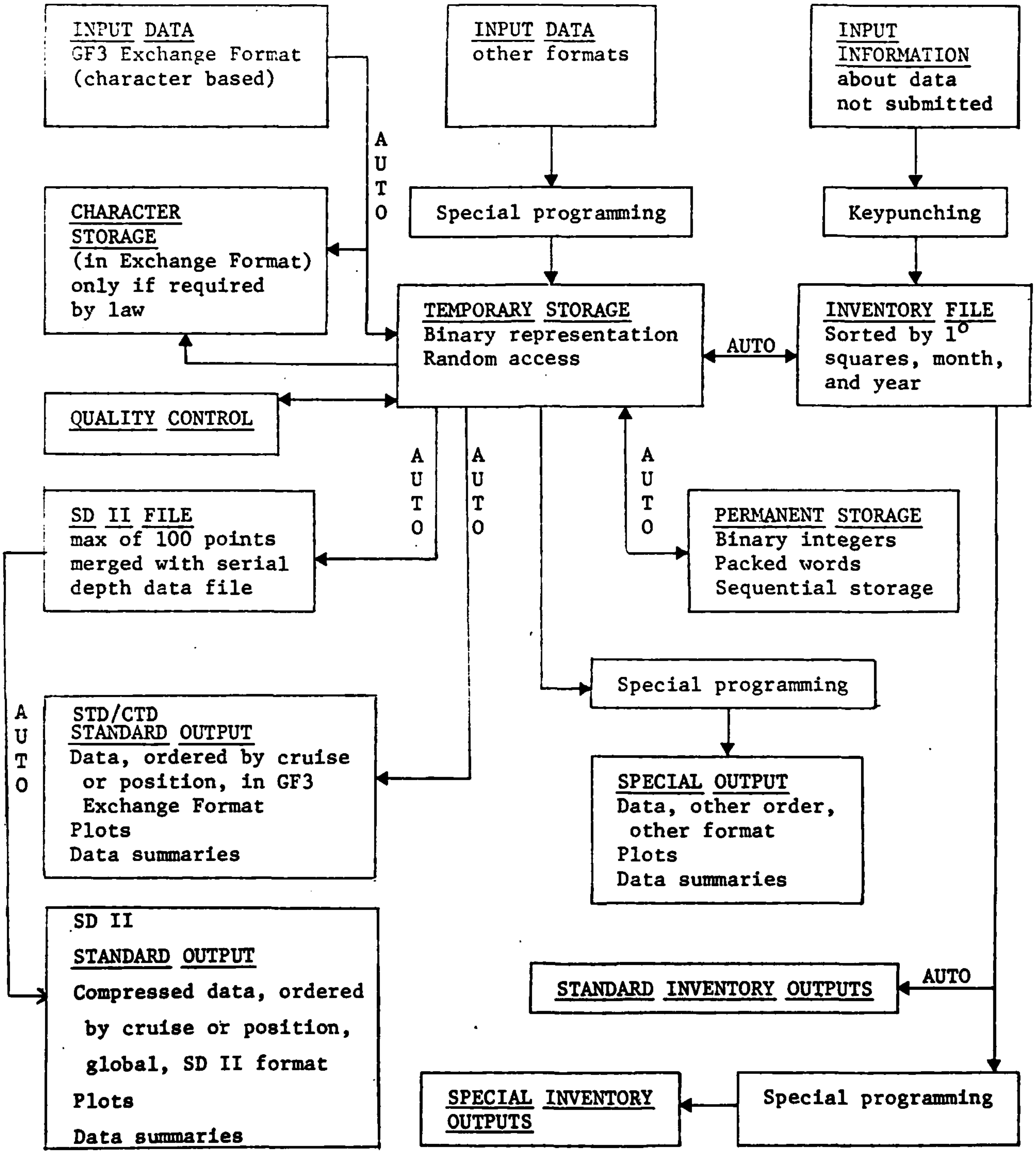


Figure 6.1

Figure 6.1

Schematic diagram of data flow through the NODC. Data flows along arrows in direction indicated assuming forms described within the boxes. Some arrows are labelled AUTO, indicating that flow along these paths can be controlled automatically by a system operator using standard programs. Only the AUTO path between the INVENTORY FILE and STANDARD INVENTORY OUTPUTS and the AUTO path between the SD II FILE and SD II STANDARD OUTPUT already exist. Some paths can only be traversed by going through "special programming" or "keypunching."

should be in a form most readily compatible to the various computers that may operate on it. This requires use of one of the character code conventions: BCD, EBCDC and ASCII.

It is recommended that the medium of exchange be digital magnetic tapes. This medium is inexpensive and very compact, as well as being highly reliable. It is, therefore, ideal for data exchange. Flexible discs should be acceptable as an alternate medium of exchange for those suppliers without digital tape drives. Many mini computers presently in common use as a part of data collection and reduction systems, use these devices.

Reading data at NODC from many different suppliers could be greatly expedited were a specified format for the character data in general use. For this reason, it is *recommended that NODC* both specify a format for data suppliers, and encourage its widespread use. NODC should still maintain the capability to read unique formats to benefit from data supplied by collectors with limited computer resources. However, all collectors should be capable of producing a recommended format if it is properly chosen. The effort required on the collectors part need be expended only once.

NODC can develop its own exchange format or adopt an existing format from some other agency or data system. One recently developed exchange format for geophysical data, GF3 (Intergovernmental Oceanographic Commission, 1979), is particularly appropriate. It has been designed for exchange between data centers. Though general

in nature so as to be able to handle meteorological soundings and station data as well as ocean profiles and moored data, instructions for implementing the format for STD/CTD data can be made more specific. Reducing the general description in the GF3 manual regarding arrangement of data to specific instructions for suppliers of STD/CTD data, simplifies their task, which encourages their rapid submission of data. This then enables NODC to read the submitted data automatically. It is recommended that NODC implement the GF3 type format to STD/CTD data exchange. It is further recommended that NODC support GF3 conversion in the community by providing software and programmers time to data supplies.

6.3 QUALITY CONTROL

For shallow waters a gross test of observation reliability can be made by comparing observed values of salinity (S) and the derived parameter, specific gravity anomaly (σ_t), to S, σ_t envelopes available from environmental models extant at NODC.

It is recommended that NODC check and flag observations that lead to density instabilities in the vertical profile, as described in Section 5.3.

It is recommended that NODC spot check each cruise by means of the noise level test described in Section 5.4. The stations used in the spot check and the results can then be recorded with each station on the cruise. The test is an objective, quantitative measure of

data reliability when it can be applied. It is expected that this test is necessary because some collectors may not quote noise levels or significant vertical resolution levels for their data because their investigations might be unaffected by these limitations.

It is suggested that NODC generate a historical potential temperature, salinity (θ ,S) relation for waters below 3000 dbars for each major ocean basin. The θ ,S curves should then be used to test the calibration of STD/CTD data on any cruise which performs measurements in any of those deep waters. The data should not be corrected by NODC. The result of the test should merely be recorded with the header information. Because of the effort in creating this standard, and its limited use, once created, this test should be considered a non essential option of an STD/CTD system.

6.4 STORAGE

This is an important issue with many possible approaches. A primary consideration is the type of requests for data, as discussed in Section 4. There are two kinds of requests. The first is for relatively low vertical resolution, on the order of 34 standard levels (see Table 4.1). When requests are made for this data, climatological phenomena are generally of interest and the data grouping required is usually by area and season (the smallest practical units being areas of one degree latitude by one degree longitude and periods of one month). The second kind of request is for the highest resolution available down to one to two

decibars. The interests here are for descriptions on the smaller space and, usually, smaller time scales. Data is preferably as synoptic as possible. Consequently, data grouped by cruise is most useful.

It is recommended, therefore, that NODC store the highest vertical resolution provided by the data suppliers in cruise order. It is also recommended that NODC "compress" the data down to 100 data cycles or less by the ICES or similar criteria discussed in Section 4. Rather than maintain it as a separate file, the compressed version of the data should be included in the extant NODC serial depth data file (in the SD II format for which 100 data cycles constitute two complete records). Once introduced to that system, geographic sorting and merging with classical hydrocasts are automatic, as are standard products. These stations should be identifiable as STD or CTD by use of a code inserted in one of the unused fields in that data system.

All classical measurements made during the STD/CTD station should be recorded with the station. There is no need to merge these measurements except when included in the serial depth file.

Because of the large amount of data that NODC potentially must store (Section 2.5) it is further recommended that NODC use as compact a storage procedure as possible for the permanent residence of the high resolution data. Data editing and display can always be done from some more convenient temporary file.

It is also recommended that NODC request from future suppliers no greater than 1 dbar vertical resolution. This is for reasons discussed in Section 4 concerning the meaning of stratification and for the sake of easier data manipulation.

It is not recommended that NODC request conductivity data because such profiles are redundant when salinity data and salinity algorithms are reported. Other measured values should be accepted. However, derived quantities such as density and dynamic height should be neither requested, accepted, nor stored.

Finally, it is recommended that NODC keep an inventory file of STD/CTD station information (including the name, address and phone number of responsible persons) for data it does not archive because of unique deployment, extra fine resolution or other reasons. Researchers looking for existing data sets can then locate them through this inventory. Stations whose data reside at NODC can also be included in the inventory.

6.5 PRODUCTS

Standard products available at minimal cost should include copies of high resolution data on magnetic tape in GF3 exchange format in either cruise or geographic order (it is expected that geographic sorts will not be global but instead will be limited in extent). Derived parameters need not be provided as users of this data product of necessity have access to computers. In lieu of the derived parameters NODC should make available on request

FORTRAN routines for the calculation of the following parameters: potential temperature (θ); salinity (S); <u>in situ</u> density (ρ); <u>in situ</u> specific volume (α); depth (Z); specific gravity anomaly (σ_t); potential specific gravity anomaly at reference pressure p (σ_p); specific volume anomaly (δ); dynamic depth (Δ D); Brunt Väisälä frequency (N); and sound velocity (SV). Test values should be supplied with every routine. For the user sans computer, listings with calculations at some coarse resolution (e.g. standard levels or ICES compression) could be provided.

Other standard products include summaries, plots and maps. Maps or listed summaries of station position (on any of the standard projections, see Table 6.1) by area, month or cruise should be available from the inventory file for all stations either reported or supplied to NODC. Such maps or listings would aid the user in selecting the cruise or cruises of interest, or deciding that a geographic sort is most suited to his needs. Plots of any parameter against any other parameter should also be available, on scales specified by the user by cruise, month or area. (Once again the assumption is that geographic sorts are limited in area). The standard parameters should be pressure, temperature, salinity and any of the derived parameters listed above.

Products not to be considered standard are geographic summaries of the profiled data (e.g., temperature at 200 m) since these are easily performed on the reduced resolution data which are channelled to the serial depth

Table 6.1

MAP PROJECTIONS AVAILABLE FROM NODC

- Mercator
- Miller
- Square
- Cylindrical Sterographic
- Lambert Equal-Area Cylindrical
- Flat-Polar Equal-Area Sinusoidal
- Equal-Area Sinusoidal
- Mollweide Homolographic
- Polar Stereographic
- Lambert Equal-Area Polar
- Colligan's Equal-Area Project of the Sphere
- Azimuthal Equidistant
- Transverse Sinusoidal
- Transverse Mollweide

Source: National Oceanographic Data Center, 1974.

data file, and because the data would be in cruise not geographic order. Special formats and customized plots also require extra programming and therefore should entail extra cost for the requestor.

Other uses of the inventory file, besides the mapping of station locations already indicated, must also be considered special requests that imply extra costs.

The system outlined for NODC here is not intended to replace the cruise data report, but is intended to be used in conjunction with it. When a data set seen in a report seems to be of interest, the reader should be able to identify it to NODC and receive a copy of the data. The archiving (e.g., on micro fiche) retrieval and dissemination of cruise data reports is a useful function of NODC not addressed by this report.

6.6 CONCLUSION

As of the spring of 1979, data submissions to NODC amounted to over 8,600 STD stations and over 45,000 CTD stations (of which over 44,000 were shallow coastal stations between Cape Hatteras and Cape May). These totals do not compare well with the order of magnitude estimate of the number of stations in existence (250,000). In general, researchers are not submitting their data to NODC.

The reasons for the lack of compliance seem to be threefold. Researchers are hesitant to put data

of uncertain quality in the public domain. Secondly, there is confusion concerning what type data NODC requires and what format to submit it in. Finally, there is a sense that submission is pointless since the data are so varied in quality, density and format that retrieval is greatly inhibited and secondary use is sharply curtailed.

The last problem should be mitigated by the implementation of a highly automated system such as described in this section. The second problem should be eliminated by publicizing the new exchange format, as recommended. The first problem requires additional efforts. It has been suggested (Ocean Science Committee *ad hoc* Panel, 1973) that NODC should document standard practices. A technical report describing standard procedures along with complete FORTRAN algorithms that perform standard processing functions, would help the user of the electronic instruments produce data in which he might have more confidence. It is recommended that NODC commission such a report and generate the appropriate algorithms.

As the oceanographic community experiences satisfactory responses to data requests, an advantageous cycle of increased supplier compliance and increased user confidence might likely be initiated.

APPENDIX A
PRESENT DATA DOCUMENTATION FORMS

		ACCESSION NUMBER	

DATA DOCUMENTATION FORM

NOAA FORM 24-13
(4-72)

U.S. DEPARTMENT OF COMMERCE
NATIONAL OCEANIC AND ATMOSPHERIC ADMINISTRATION
NATIONAL OCEANOGRAPHIC DATA CENTER
RECORDS SECTION
ROCKVILLE, MARYLAND 20852

FORM APPROVED
OMB No. 41-R[illegible]

This form should accompany all data submissions to NODC. Section A, Originator Identification, must be completed when the data are submitted. It is highly desirable for NODC to also receive the remaining pertinent information at that time. This may be most easily accomplished by attaching reports, publications, or manuscripts which are readily available describing data collection, analysis, and format specifics. Readable, handwritten submissions are acceptable in all cases. All data shipments should be sent to the above address.

A. ORIGINATOR IDENTIFICATION

THIS SECTION MUST BE COMPLETED BY DONOR FOR ALL DATA TRANSMITTALS

1. NAME AND ADDRESS OF INSTITUTION, LABORATORY, OR ACTIVITY WITH WHICH SUBMITTED DATA ARE ASSOCIATED

2. EXPEDITION, PROJECT, OR PROGRAM DURING WHICH DATA WERE COLLECTED

3. CRUISE NUMBER(S) USED BY ORIGINATOR TO IDENTIFY DATA IN THIS SHIPMENT

4. PLATFORM NAME(S)	5. PLATFORM TYPE(S) *(E.G., SHIP, BUOY, ETC.)*	6. PLATFORM AND OPERATOR NATIONALITY(IES)		7. DATES	
		PLATFORM	OPERATOR	FROM: MO/DAY/YR	TO: MO/DAY/YR

8. ARE DATA PROPRIETARY?

☐ NO ☐ YES

IF YES, WHEN CAN THEY BE RELEASED FOR GENERAL USE? YEAR____ MONTH____

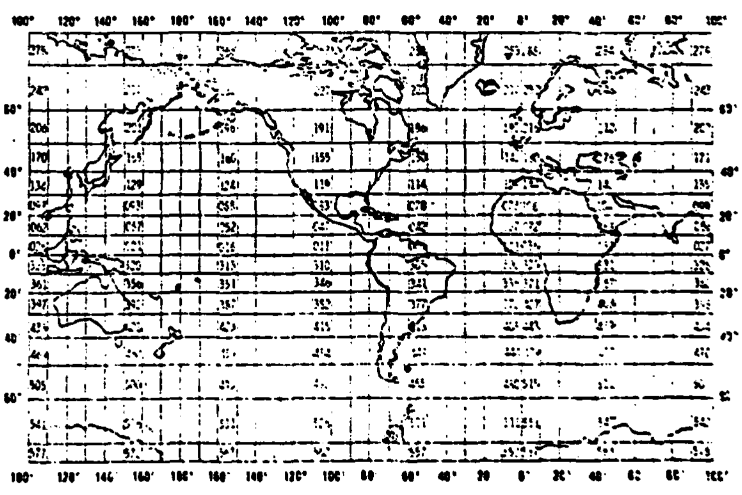
9. ARE DATA DECLARED NATIONAL PROGRAM (DNP)?
(I.E., SHOULD THEY BE INCLUDED IN WORLD DATA CENTERS HOLDINGS FOR INTERNATIONAL EXCHANGE?)

☐ NO ☐ YES ☐ PART *(SPECIFY BELOW)*

10. PERSON TO WHOM INQUIRIES CONCERNING DATA SHOULD BE ADDRESSED WITH TELEPHONE NUMBER *(AND ADDRESS IF OTHER THAN IN ITEM-1)*

11. PLEASE DARKEN ALL MARSDEN SQUARES IN WHICH ANY DATA CONTAINED IN YOUR SUBMISSION WERE COLLECTED.

GENERAL AREA



NOAA FORM 24-13

USCOMM-DC 44283-P72

B. SCIENTIFIC CONTENT

Include enough information concerning manner of observation, instrumentation, analysis, and data reduction routines to make them understandable to future users. Furnish the minimum documentation considered relevant to each data type. Documentation will be retained as a permanent part of the data and will be available to future users. Equivalent information already available may be substituted for this section of the form (i.e., publications, reports, and manuscripts describing observational and analytical methods). If you do not provide equivalent information by attachment, please complete the scientific content section in a manner similar to the one shown in the following example.

EXAMPLE (HYPOTHETICAL INFORMATION)

NAME OF DATA FIELD	REPORTING UNITS OR CODE	METHODS OF OBSERVATION AND INSTRUMENTS USED (SPECIFY TYPE AND MODEL)	ANALYTICAL METHODS (INCLUDING MODIFICATIONS) AND LABORATORY PROCEDURES	DATA PROCESSING TECHNIQUES WITH FILTERING AND AVERAGING
Salinity	‰	Nansen bottles	Inductive salinometer (Hytech model S510)	N/A (Not applicable)
		STD Bissett-Berman Model 9006	N/A	Values averaged over 5-meter intervals
Water color	Forel scale	Visual comparison with Forel bottles	N/A	N/A
Sediment size	ϕ units and percent by weight	Ewing corer	Standard sieves. Carbonate fraction removed by acid treatment	Same as "Sedimentary Rock Manual," Folk '65

(SPACE IS PROVIDED ON THE FOLLOWING TWO PAGES FOR THIS INFORMATION)

B. SCIENTIFIC CONTENT

NAME OF DATA FIELD	REPORTING UNITS OR CODE	METHODS OF OBSERVATION AND INSTRUMENTS USED (SPECIFY TYPE AND MODEL)	ANALYTICAL METHODS (INCLUDING MODIFICATIONS) AND LABORATORY PROCEDURES	DATA PROCESSING TECHNIQUES WITH FILTERING AND AVERAGING

NOAA FORM 24-13 (2-72)

USCOMM-DC 41289-P

C. DATA FORMAT

This information is requested only for data transmitted on punched cards or magnetic tape. Have one of your data processing specialists furnish answers either on the form or by attaching equivalent readily available documentation. Identify the nature and meaning of all entries and explain any codes used.

1. List the record types contained in your file transmittal (e.g., tape label record, master, detail, standard depth, etc.).

2. Describe briefly how your file is organized.

3-13. Self-explanatory.

14. Enter the field name as appropriate (e.g., header information, temperature, depth, salinity.

15. Enter starting position of the field.

16. Enter field length in number columns and unit of measurement (e.g., bit, byte, character, word) in unit column.

17. Enter attributes as expressed in the programming language specified in item 3 (e.g., "F 4.1," "BINARY FIXED (5.1)").

18. Describe field. If sort field, enter "SORT 1" for first, "SORT 2" for second, etc. If field is repeated, state number of times it is repeated.

C. DATA FORMAT

COMPLETE THIS SECTION FOR PUNCHED CARDS OR TAPE, MAGNETIC TAPE, OR DISC SUBMISSIONS.

1. LIST RECORD TYPES CONTAINED IN THE TRANSMITTAL OF YOUR FILE
   GIVE METHOD OF IDENTIFYING EACH RECORD TYPE

2. GIVE BRIEF DESCRIPTION OF FILE ORGANIZATION

3. ATTRIBUTES AS EXPRESSED IN ☐ PL-1 ☐ ALGOL ☐ COBOL ☐ FORTRAN ☐ ________ LANGUAGE

4. RESPONSIBLE COMPUTER SPECIALIST:
   NAME AND PHONE NUMBER ________
   ADDRESS ________

COMPLETE THIS SECTION IF DATA ARE ON MAGNETIC TAPE

5. RECORDING MODE ☐ BCD ☐ BINARY ☐ ASCII ☐ EBCDIC ☐ ________	9. LENGTH OF INTER-RECORD GAP (IF KNOWN) ☐ 3/4 INCH ☐ ________
6. NUMBER OF TRACKS (CHANNELS) ☐ SEVEN ☐ NINE ☐ ________	10. END OF FILE MARK ☐ OCTAL 17 ☐ ________
7. PARITY ☐ ODD ☐ EVEN	11. PASTE-ON-PAPER LABEL DESCRIPTION *(INCLUDE ORIGINATOR NAME AND SOME DAY SPECIFICATIONS OF DATA TYPE, VOLUME NUMBER)*
8. DENSITY ☐ 200 BPI ☐ 1600 BPI ☐ 556 BPI ☐ 800 BPI ☐ ________	12. PHYSICAL BLOCK LENGTH IN BYTES
	13. LENGTH OF BYTES IN BITS

NOAA FORM 24-13 USCOMM-DC 44289-P72

RECORD FORMAT DESCRIPTION

RECORD NAME ______

14. FIELD NAME	15. POSITION FROM 1 MEASURED IN ______ (e.g., bits, bytes)	16. LENGTH NUMBER	16. LENGTH UNITS	17. ATTRIBUTES	18. USE AND MEANING

NOAA FORM 24-13

USCOMM-DC 44283-P72

D. INSTRUMENT CALIBRATION

This calibration information will be utilized by NOAA's National Oceanographic Instrumentation Center in their efforts to develop calibration standards for voluntary acceptance by the oceanographic community. *Identify the instruments used by your organization to obtain the scientific content of the DDF* (i.e., STD, temperature and pressure sensors, salinometers, oxygen meters, velocimeters, etc.) and furnish the calibration data requested by completing and/or checking ("✓") the appropriate spaces. Add the interval time (i.e., 3 months, 6 months, 9 months, etc.) if the fixed interval calibration cycle is checked.

INSTRUMENT TYPE (MFR., MODEL NO.)	DATE OF LAST CALIBRATION	INSTRUMENT WAS CALIBRATED BY		CHECK ONE: INSTRUMENT IS CALIBRATED					INSTRUMENT IS NOT CALIBRATED (√)
		YOUR ORGANIZATION (√)	OTHER ORGANIZATION (GIVE NAME)	AT FIXED INTERVALS (√)	BEFORE OR AFTER USE (√)	BEFORE AND AFTER USE (√)	ONLY AFTER REPAIR (√)	ONLY WHEN NEW (√)	

NOAA FORM 24-13

USCOMM-DC 44289-P72

APPENDIX B

PROPOSED DATA DOCUMENTATION FORM, PART A

Existing form is recommended with the addition of the following items:

Purpose of cruise

Estimate of percent data loss in profiles sent to NODC

Independent variable
time, pressure or other (specify)

Standardization parameters reported

PROPOSED DATA DOCUMENTATION FORM, PART B

1. PARAMETER:______________________ Independent Variable ☐

2. a. Units:____

   b. Target Accuracy:______________________________________

3. SENSOR MANUFACTURER AND MODEL AND SERIAL NUMBER(S):

   ____

4. DATA LOGGING:

   a. Manufacturer and Model and Serial Number(s):

      ____

   b. Technique (i.e., period counting, frequency counting, etc.):

      ____

   c. Raw Data Sampling:

      i. Sample interval: ______________________________

      ii. Sample rate: ______________________________

5. DEPLOYMENT

   a. Coupled to platform pitch and roll?

      YES ☐ , NO ☐ (If "No" go to c)

   b. Range of ship roll periods:___________to_____________

   c. Typical descent rate: high gradient: _____________
                            low gradient: _____________

   d. Trace Reported:

      downtrace only ☐ uptrace only ☐

      either one, only ☐ both, separately ☐

      both, averaged ☐ other ☐ ,

      specify: ____

      ____

6. TIME LAG CORRECTION

a. Performed? YES ☐ , NO ☐ (If "No" go to 7)

b. Indicate sequence of this step:______________________

____

c. Performed on time series?

YES ☐, NO ☐ (If "Yes go to e)

d. Performed on series of another independent parameter. Name parameter:__________________________

____

e. Algorithm (Give reference, define variables)

7. DERIVATIONS

a. Is Parameter directly observable (i.e., not derived from other observables)?

YES ☐ , NO ☐ (If "Yes" go to 8)

b. Indicate sequence of this step:______________________

____

c. Is derivation by analog computation?

YES ☐, NO ☐

d. Is derivation by digital computation?

YES ☐, NO ☐

e. Algorithm (Give reference, define variables)

8. EDITING

a. Is any editing employed to remove suspect points?

YES ☐ , NO ☐ (If "No" go to 9)

b. Indicate sequence of this step:____________________

____

c. Is editing performed manually?

YES ☐ , NO ☐ (If "Yes" go to f)

d. Editing is performed automatically.

i. Absolute limits tested?

YES ☐ , NO ☐ , Range:________to______________

ii. Incremental limits tested?

YES ☐ , NO ☐ , Range:_________to___________

iii. Other procedure used?

YES ☐ , No ☐ , (If "No" go to f)

e. Algorithm (Give reference, define variables)

f. (Only if this is the independent parameter)

i. Are non monotonic changes deleted?

YES ☐ , NO ☐ , (If "No" go to 9)

ii. Algorithm (Give reference, define variables)

9. SMOOTHING

a. Is any smoothing or averaging performed?

YES ☐ , NO ☐ (If "No" go to 10)

b. Indicate sequence of this step:____________________

c. Performed on time series?

YES ☐ , NO ☐ (If "Yes" go to e)

d. Performed on series of another independent parameter.

Name parameter:____________________________________

e. Algorithm (Give reference, define variables)

10. CALIBRATION

a. Is any calibration procedure employed for this data?

YES ☐ , NO ☐ (If "No" go to 11)

b. Is any laboratory calibration performed.

YES ☐ , NO ☐ (If "No" go to d)

c. Indicate sequence of this step:____________________

i. Installation:______________________________

ii. Date:_____________________________________

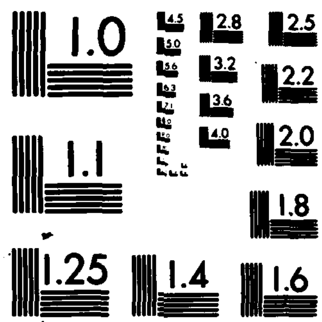
iii. Standard:_________________________________

(If temperature, IPTS '48 ☐ or IPTS '68 ☐)

iv. Results:__________________________________

AD-A091 864 SCIENCE APPLICATIONS INC MCLEAN VA F/G 8/10
REQUIREMENTS FOR AN HISTORICAL STRATIFICATION FILE USING STD AN--ETC(U)
JUN 80 E J MOLINELLI, A D KIRWAN N00014-79-C-0906
UNCLASSIFIED SAI-81-179-WA NL

END
DATE
FILMED
81-1
DTIC


1.0
1.1
1.25
1.4
1.6
1.8
2.0
2.2
2.5
2.8
3.2
3.6
4.0
4.5
5.0
5.6
6.3

d. Are water bottle (reversing thermometer) comparisons made?

YES ☐ , NO ☐ (If "No" go to h)

e. Indicate sequence of this step:________________

f. How are bottles deployed?

i. Separate lowering ☐
ii. Same lowering ☐ Give spacings from STD/CTD:

____

iii. Command sampling ☐ Give distance from STD/CTD: and indicate uptrace or downtrace:

____

iv. Other ☐ Describe:________________

____

v. Derivation of water bottle measurement. Algorithm (give references & define variables)

____

g. How are comparisons used?

i. Number of comparisons per "calibration"

point:________________

ii. Results of comparison:________________

____

iii. Are data corrected by these results?

YES ☐ , NO ☐

h. Are other techniques used (e.g., historical potential temperature, salinity correlations)?

YES ☐ , NO ☐ (If "No" go to 11)

i. Indicate sequence of this step:____________________

j. Specify technique (Give references)

k. Results
   i. What were the results of the implemented techniques:____________________

   ____

   ii. Are data corrected by these results?

   YES ☐ , NO ☐

11. INTERPOLATION

a. Are any points for this parameter interpolated?

YES ☐ , NO ☐ (If "No" skip rest)

b. Indicate sequence of this step:____________________

____

c. Algorithm (Give reference, define variables)

d. Are interpolated points indicated?

YES ☐ , NO ☐

e. If so, how?:____________________

____

PROPOSED DATA DOCUMENTATION FORM, PART C

No changes to existing form recommended at this time.

This form to be replaced by use of a standardized application of GF3.

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